



## Chemical constituents of *Solanum coagulans* and their antimicrobial activities

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**[ABSTRACT]** The present study aimed at determining the chemical constituents of *Solanum coagulans* and their antimicrobial activities. The compounds were isolated by various chromatographic techniques and their structures were elucidated on the basis of extensive spectroscopic analysis, chemical methods, and comparison with reported spectroscopic data. One new phenolic glycoside, methyl salicylate 2-*O*- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-glucopyranoside (**1**), together with 12 known compounds (**2–13**), were isolated from the aerial parts of *Solanum coagulans*. Compound **1** was a new phenolic glycoside, and **2–6** were isolated from *Solanum* genus for the first time. The antimicrobial activities of the isolated compounds were also evaluated. Compound **7** showed remarkable antifungal activity against *T. mentagrophytes*, *M. gypseum* and *E. floccosum* with MIC values being 3.13, 1.56 and 3.13  $\mu\text{g}\cdot\text{mL}^{-1}$ , respectively.

**[KEY WORDS]** *Solanum coagulans*; chemical constituents; antimicrobial activity

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### Introduction

*Solanum* is an important genus of Solanaceae family, which is widely distributed in the regions from temperate zone to the tropics<sup>[1]</sup>. Previous phytochemical investigations on the genus *Solanum* have demonstrated that it is a fertile source of steroidal glycosides<sup>[2–4]</sup> and steroidal alkaloid glycosides<sup>[5–7]</sup>. *Solanum coagulans* Forsk is an herb or shrub and often used in folk medicine for the treatment of edema, rheumatic arthritis, and toothache. However, the chemical constituents and biological activities of this species have not been reported so far. In the course of searching for new and

bioactive chemical constituents from Chinese folk medicines<sup>[8–10]</sup>, the phytochemical and antimicrobial investigation on the aerial parts of the species was performed. In the present study, one new phenolic glycoside, methyl salicylate 2-*O*- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 2)- $\beta$ -D-glucopyranoside (**1**), together with 12 known ones (**2–13**), was isolated. Herein, we report the isolation, structural elucidation, and evaluation for the antimicrobial activity of these compounds.

### Results and Discussion

The MeOH extract of the aerial parts of *S. coagulans* was suspended in water and then partitioned with EtOAc and *n*-BuOH. The *n*-BuOH soluble material was subjected to repeated column chromatography (CC) on silica gel and reversed phase silica gel column to afford compounds **1–13** (Fig. 1).

Compound **1** was obtained as a white amorphous powder. Its molecular formula was determined to be  $\text{C}_{20}\text{H}_{28}\text{O}_{13}$  on the base of the quasi-molecular ion at  $m/z$   $[\text{M}]^+$  476.153 6 (calcd. for  $\text{C}_{20}\text{H}_{28}\text{O}_{13}$ , 476.153 0) in HR-EI-MS and  $^{13}\text{C}$  NMR data, representing seven indices of hydrogen deficiency. The UV (MeOH) spectrum of compound **1** exhibited maximal absorpt-

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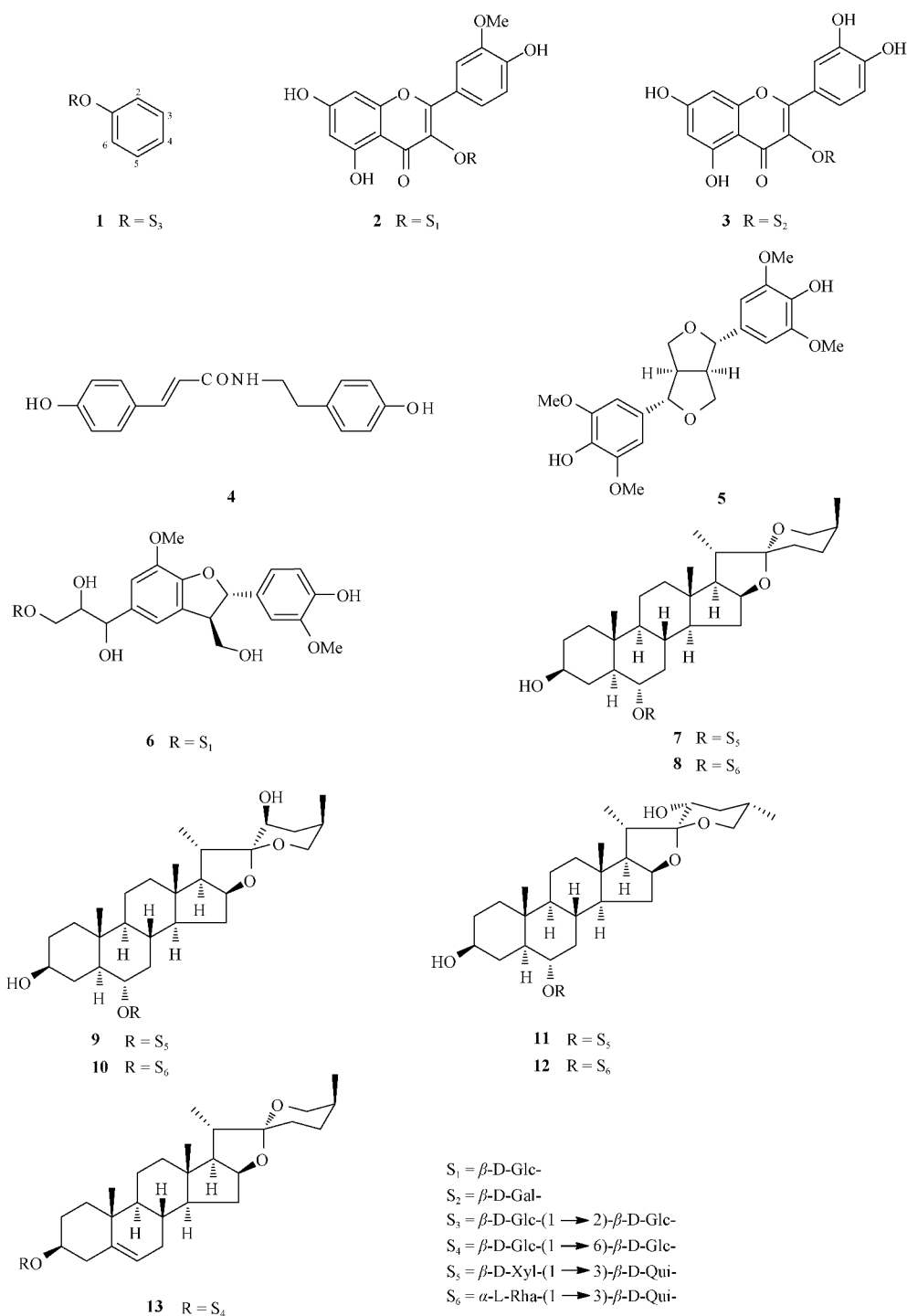


Fig. 1 Structures of compounds 1–13

ion bands at 204, 228, and 290 nm, suggesting the presence of an aromatic ring. Its IR spectrum revealed the presence of hydroxyl (3 429 cm<sup>-1</sup>), an ester carbonyl (1 716 cm<sup>-1</sup>) and aromatic (1 631, 1 491 and 1 453 cm<sup>-1</sup>) functionalities. The <sup>1</sup>H NMR spectrum (Table 1) displayed signals for four aromatic protons at δ<sub>H</sub> 7.77 (1H, d, *J* = 7.7 Hz, H-3), 7.51 (1H, t, *J* = 7.4 Hz, H-5), 7.25 (1H, d, *J* = 8.5 Hz, H-6), and 7.06 (1H, t, *J* = 7.5 Hz, H-4), one methoxyl protons at δ<sub>H</sub> 3.87 (3H,

s), and two anomeric protons at δ<sub>H</sub> 5.34 (1H, d, *J* = 7.4 Hz) and 4.82 (1H, d, *J* = 7.8 Hz). The <sup>13</sup>C NMR and DEPT spectra of compound 1 showed 20 carbon signals, 8 of which were assigned to the aglycone moiety, including those corresponding to one methoxyl carbon at δ<sub>C</sub> 52.6, one carbonyl carbon at δ<sub>C</sub> 167.9 (C-7), one oxy-bearing aromatic carbon at δ<sub>C</sub> 157.6 (C-1), four aromatic methine at δ<sub>C</sub> 134.9 (C-5), 132.4 (C-3), 122.5 (C-4), and 116.2 (C-6), and one

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