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A New Cycloartane Triterpene Glycoside from *Souliea vaginata*

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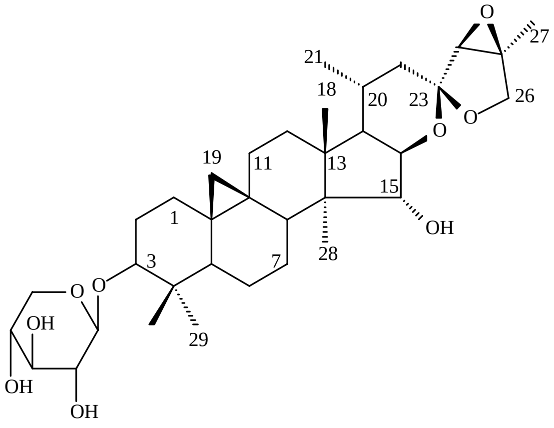
Abstract: A new cycloartane triterpene glycoside was isolated from the rhizome of *Souliea vaginata*. Its structure was established as 12-deacetyloxy-15α-hydroxy-23-*epi*-26-deoxyactein by spectroscopic and chemical methods.

Keywords: *Souliea vaginata*, ranunculaceae, cycloartane, triterpene glycosides.

Souliea vaginata (Maxim.) Franch. (Ranunculaceae) is widely distributed in the southwest and northwest of China. It possesses anti-inflammatory analgesic functions as a well-known Chinese folk medicine. Its rhizomes or the whole plant are used to treat conjunctivitis, stomatitis, pharyngitis, enteritis, and diarrhea[1]. Previously, we have reported the isolation and structural elucidation of suolieasides A-C from the ethanol extract of the rhizomes of this plant[2]. In our further investigation on the same plant, a new cycloartane triterpene glycoside (**1**, **Figure 1**) has been isolated, and its structure was established on the basis of the spectroscopic methods and chemical reactions.

Figure 1 Structure of compound **1**



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Compound **1** was isolated as colorless needles and exhibited positive Libermann-Burchard reaction and Molish reaction. Its molecular formula was determined as $C_{35}H_{54}O_9$ from the positive HR-FAB-MS, showing a $[M+Na]^+$ ion peak at *m/z* 641.3640 (Calcd. 641.3666). In the ^{1}H-NMR spectrum (**Table 1**) the cyclopropane methylene signals of **1** were observed at δ 0.25 and 0.49 (d, each 1H, J = 3.5 Hz) and the spectrum also showed six methyl groups at δ 0.95 (d, J = 6.0 Hz), 1.02 (s), 1.24 (s), 1.29 (s), 1.30 (s), 1.41 (s). The ^{13}C-NMR spectra (**Table 1**) of **1 s**howed five oxygenated carbons assignable to the sugar moiety [δ 107.5 (C-1′), 75.6 (C-2′), 78.6 (C-3′), 71.3 (C-4′), 67.1 (C-5′)] and the sugar was indentified as D-xylose by acid hydrolysis followed by HPLC analysis with an authentic sample and its configuration was elucidated as β according to the coupling constants of H-1′ (J = 7.5 Hz). Futhermore, the ^{13}C-NMR spectra of **1** also showed the signals ascribed to four oxygen-bearing methine carbons at δ 88.5 (C-3), 84.2 (C-15), 83.9 (C-16) and 62.4 (C-24), one oxygen-bearing methylene carbon at δ 68.0 (C-26), and two oxygen-bearing quaternary methylene carbon at δ 106.4 (C-23) and 62.1 (C-25). The spectral data of **1** showed a very close similarity to those of 26-deoxyactein[3], and also suggested **1** was a highly oxygenated 9, 19-cycloartane triterpene monoglycoside with the same skeleton as 26-deoxyactein.

Table 1 ^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) data of **1** (in pyridine-d_5 δ in ppm)

Position	δ_H (J in Hz)	δ_C	Position	δ_H (J in Hz)	δ_C
1	1.17, 1.58	32.5	21	0.95 d (6.0)	20.3
2	1.94, 2.35	30.2	22	1.34, 1.55	37.7
3	3.49 dd (3.5, 11.5)	88.5	23		106.4
4		41.4	24	3.50 s	62.4
5	1.34	47.5	25		62.1
6	0.65, 1.45	21.1	26	3.57 d (10.5), 4.03 d (10.5)	68.0
7	1.06, 2.15	26.2	27	1.41 s	14.2
8	1.75	48.9	28	1.24 s	12.7
9		20.7	29	1.30 s	25.7
10		26.6	30	1.02 s	15.4
11	1.24, 2.10	26.3	1′	4.85 d (7.5)	107.5
12	1.55 (2H)	34.1	2′	4.01 t (8.0)	75.6
13		44.6	3′	4.15 t (8.0)	78.6
14		48.0	4′	4.23	71.3
15	4.42 d (4.0)	84.2	5′	3.74 t (10.5), 4.35 dd, (5.0, 11.5)	67.1
16	4.10 dd (4.0, 10.5)	83.9			
17	1.73 d (10.5)	54.9			
18	1.29 s	20.9			
19	0.25 d (3.5), 0.49 d (3.5)	30.6			
20	2.19	23.5			

The ^{1}H-NMR spectrum showed that **1** possesses an ABX-type spin system of three methine proton signals (H-15, 16 and 17). The ^{1}H-^{1}H COSY spectrum of **1** showed cross peaks between the signal at δ 4.10 (dd, J = 10.5, 4.0 Hz, H-16) and two methine signals at δ 4.42 (d, J = 4.0 Hz, H-15) and δ 1.73 (d, J = 10.5 Hz, H-17). In the HMQC spectrum of **1**, the proton signals due to H-15, 16 and 17 were correlated with the carbon signals at δ 84.2, 83.9 and 54.9 ppm, respectively. Thus, the hydroxyl group in **1** was located at C-15. This result was also supported by the HMBC correlations between C-15/CH$_3$-28, C-28/H-15 and C-14/H-15. In the NOESY spectrum of **1**, significant cross peaks between H-15/H-18, H-16/H-28, H-16/H-17, H-3/H-29 and H-3/H-1′ were observed, which enabled the establishment of 15α-OH and 3 β-OH. According to the literature[3], when the configuration of epoxy between C-23 and C-26 is α-oriented, C-16 and C-20 were observed at δ 73.0 and 26.0 ppm; on the contrary, C-16 and C-20 were observed at δ 74.5 and 23.3 ppm, respectively. According to the chemical shifts of C-16 and C-20, the orientation of epoxy between C-23 and C-26 is assigned as β. Therefore, compound **1** was elucidated as 12-deacetyloxy-15α-hydroxy-23-*epi*-26-deoxyactein.

Acknowledgments

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