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A New Triterpenoid Glycoside from *Dichotomanthes tristaniaecarpa*

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Abstract: A new triterpenoid glycoside **1**, 1β, 2α, 3α, 19α-tetrahydroxyurs-12-en-28-oic acid β-D glucopyranosyl ester was isolated from *Dichotomanthes tristaniaecarpa.* The structure was elucidated on the basis of spectral means.

Keywords: Triterpenoid glucoside, *Dichotomanthes tristaniaecarp*, Rosaceae.

Dichotomanthes tristaniaecarp (Kurz.) belongs to the family Rosaceae. Its root bark is used as Chinese folk medicine for treatment of flu, cough, sore throat and nosebleed. Chemical constituents of this species have not been reported previously.

Compound **1** was obtained as colorless needles, mp. 213-215 °C. The molecular formula was determined as $C_{36}H_{58}O_{11}$ by its negative-ion FAB MS ($[M]^-$ at *m/z* 665) and ^{13}C NMR DEPT spectrum. The analysis of ^{13}C NMR spectrum showed 30 signals for the aglycone, consistent with a triterpenoid structure. A singlet at δ 2.91 in the ^1H NMR spectrum, which is characteristic for the H-18 of ursane triterpenoid with 19α-hydroxyl substitution, and a pair of double bond signals at δ 130.0 (C-12) and 138.2 (C-13) in the ^{13}C NMR spectrum, suggested a 19α-hydroxyurs-12-en skeleton [1]. Three oxygenated methines in the ^{13}C NMR spectrum were attributed to C-1, C-2, C-3 by analysis of ^1H-^1H COSY, HMQC, HMBC data (**Figure 1**). In the ROESY spectrum, the correlation between H-1 and H-5 indicated that both protons were located at the same side of A-ring. The coupling constants between H-1 (d, J = 9.4Hz) and H-2 (d, J = 9.4Hz) confirmed that H-1 and H-2 were both axial with α and β-configuration respectively. H-3 showing a broad singlet in the ^1H NMR spectrum, inferred that H-3 was equatorial with β configuration. This was confirmed by the fact that H-3 correlated to both H-23 and H-24 in the NOESY spectrum. Correspondingly, the three hydroxyls were located at 1β, 2α, 3α respectively. The sugar moiety was identified as β-D glucosyl by comparison with reported data[1, 2]. H-1' exhibited a HMBC cross peak to C-28, confirming that the glucosyl group was linked to C-28 (**Figure 1**). Thus, **1** was elucidated as 1β, 2α, 3α, 19α-tetrahydroxyurs-12-en-28-oic acid β-D-glucopyranosyl ester. The assignments of ^1H and ^{13}C NMR data are given in **Table 1** and **2**.

Table 1. ^{13}C NMR (100 MHz) data of **1** (δ in ppm)*

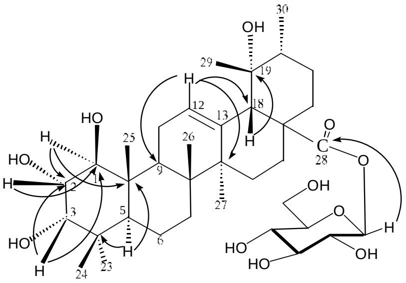
Position		Position		Position		Position		Position		Position	
1	81.0	7	33.9	13	138.2	19	72.8	25	13.1	1'	95.9
2	71.5	8	41.5	14	42.2	20	42.2	26	18.0	2'	74.1
3	79.8	9	48.6	15	29.4	21	28.1	27	24.7	3'	79.0
4	38.5	10	43.9	16	26.8	22	37.7	28	177.0	4'	71.5
5	48.7	11	26.3	17	48.8	23	29.4	29	27.0	5'	79.2
6	19.0	12	130.0	18	54.4	24	22.4	30	16.7	6'	62.6

Table 2. ^{1}H NMR (400 MHz) data of **1** (δ in ppm, J in Hz)*

Position		Position		Position		Position	
H-1'	6.30 (d, 6.5)	H-3	3.85 (br.s)	Me-23	1.22 (s)	Me-27	1.69 (s)
H-1	4.11 (d, 9.4)	H-12	5.64 (d, 3.4)	Me-24	0.93 (s)	Me-29	1.35 (s)
H-2	4.16 (d, 9.4)	H-18	2.91 (s)	Me-25, 26	1.31 (s)	Me-30	1.04 (d, 6.6)

*The data were measured in pyridine-d_5 with TMS as internal standard (**Table 1** and **2**).

Figure 1. Selected HMBC for **1**



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