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A New Phytosterone from *Passiflora wilsonii*

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Abstract: A new phytosterone named passionsterone **1** has been isolated from the roots of *Passiflora wilsonii*, along with the known compound 24R-ethyl-5 α -cholestane-3 β ,6 α -diol **2**. The structure of passionsterone **1** was elucidated as 24R-ethyl-5 α -cholestane-3 β ,6 α -diol-23-one by spectroscopic means.

Keyword: *Passiflora wilsonii*, passionsterone.

Passiflora wilsonii, a traditional folk medicine, has been used in the minority of Yunnan province[1]. In the previous paper, we reported the isolation of six known triterpenoids and steroids from the roots of *Passiflora wilsonii*[2]. Further purification of the remaining fractions by silica gel afforded two steroids, one is the known compound 24R-ethyl-5α-cholestane-3β, 6α-diol **2**, the other is a new phytosterone named passionsterone **1**.

Compound **1** was obtained as colorless needles, mp: 127-129℃. Its IR spectrum (KBr) exhibited the carbonyl absorption (1712 cm^{-1}). Its ^{1}H-NMR (δ ppm) spectrum showed signals at 3.65 (m,1H) and 3.40 (dt,1H, J=4.45 and 10.65Hz), which are characteristic for H-3 and H-6, respectively, for 3 β , 6 α -dihydroxysteroid[3]. The methyl signals at 0.671 (s,3H, Me-18), 0.786 (t,3H, J=7.5 Hz, Me-29), 0.789 (s,3H, Me-19), 0.839 (d,3H, J=6.7 Hz, Me-26), 0.841 (d,3H, J=6.7 Hz, Me-27) and 0.896 (d,3H, J=6.5 Hz, Me-21) indicated the 24R configuration of the sterol[4~5].

Comparison of the ^{13}C-NMR of **1** and **2** showed (**Table 1**) that **1** differs structurally from **2** only in the side chain (C-20－C-29), one carbonyl signal at 214.5 ppm appears in compound **1.** The regiochemistry of these side chain carbons was established from ^{1}H-^{1}H COSY, HMQC and HMBC experiments. The long-range correlations between H_3-21 and C-22, H-22 and C-17, H-25 and C-23, H_2-28 and C-23 established the presence of carbonyl at the C-23 position. The γ –gauche effects at C-20 and C-28 is also evident.

The HR-ESI-MS suggested that the molecular mass for $C_{29}H_{51}O_3$ [M+H] (calcd. 447.3838, found 447.3829). The characteristic peaks in EI-MS appeared at *m/z* 446 $[M]^+$, 428 [M-H_2O], 361 [M-C_6H_{13}], 343 [M-C_6H_{13}-H_2O], 318 [base peak, M-$C_8H_{16}O$], 300 [M-$C_8H_{16}O$-H_2O], 289 [M-$C_{10}H_{21}O$], 271 [M-$C_{10}H_{21}O$-H_2O]. The base peak at *m/z*

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318, which is the fragment of McLafferty rearrangement, confirmed the carbonyl at the C-23 position. Therefore, the structure of compound **1** was elucidated as 24R-ethyl-5α-cholestane-3β, 6α-diol-23-one.

Figure 1 The structure and key HMBC of compound **1** (H→C)

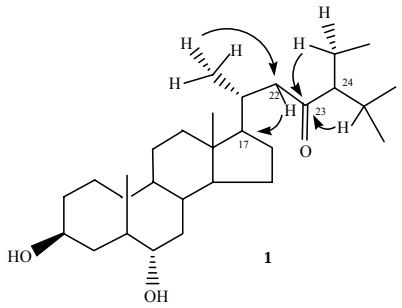

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Table 1 ^{13}C-NMR data of compound **1** and **2** (75 MHz, $CDCl_3$ δ ppm)

	1	**2**		**1**	**2**
Carbon	δ_c	δ_c	Carbon	δ_c	δ_c
1	37.3 t	37.3 t	16	28.4 t	28.2 t
2	31.1 t	31.1 t	17	55.8 d	56.2 d
3	71.3 d	71.3 d	18	12.1 q	12.1 q
4	32.3 t	32.3 t	19	13.5 q	13.4 q
5	51.8 d	51.7 d	20	31.7 d	36.1 d
6	69.5 d	69.5 d	21	20.1 q	18.7 q
7	41.7 t	41.7 t	22	51.0 t	33.9 t
8	34.3 d	34.3 d	23	214.5 s	26.1 t
9	53.8 d	53.8 d	24	60.9 d	45.8 d
10	36.3 s	36.3 s	25	29.2 d	29.2 d
11	21.2 t	21.2 t	26	21.2 q	19.7 q
12	39.8 t	39.8 t	27	19.7 q	19.0 q
13	42.8 s	42.6 s	28	21.6 t	22.7 t
14	56.3 d	56.1 d	29	11.9 q	12.0 q
15	24.2 t	24.2 t			

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