Chinese Chemical Letters Vol. 13, No. 3, pp 253 –255, 2002
http://www.imm.ac.cn/journal/ccl.html

Two New Triterpenoid Glycosides from *Elsholtzia bodinieri* Van′t

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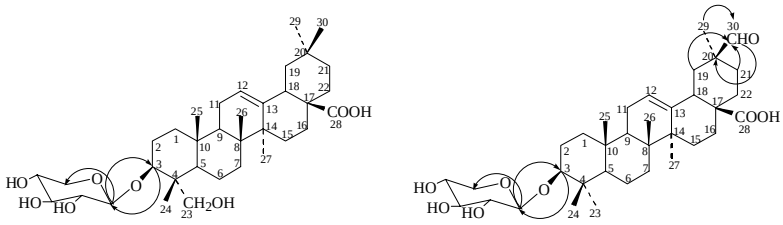
Abstract: Two new triterpenoid glycosides, hederagenin-3-*O*-β-D-xylopyranoside (**1**), dodecandral 3-*O*-β-D-xylopyranoside(**2**), were isolated from *Elsholtzia bodinieri* Van′t. The structures of **1** and **2** were established by spectroscopic and chemical methods.

Keywords: Hederagenin xyloside, *Elsholtzia bodinieri*, Labiatae.

Elsholtzia bodinieri Van′t (Labiatae) named Feng-Wei-Cha or Dong-Zi-Su, is a Chinese medicinal plant, which is distributed in Yunnan and Guizhou Province of China. It is used in treatment of cough, headache, pharyngitis, fever and heptatitis[1]. In order to seek for the relative bioactive components, we studied the chemical constituents of *E. bodinieri*, which have not been reported in the literature. Two new triterpenoid glycosides, hederagenin-3-*O*-β-D-xylopyranoside (**1**), dodecandral-3-*O*-β-D-xylopyranoside (**2**), and the aglycone, hederagenin (**3**)[2], were obtained from the ethanol extracts of the aerial parts of this plant.

Figure 1 The structures and key HMBC of **1** and **2** (H→C)



1 **2**

Compound **1** and **2** obtained as crystal solids, $[\alpha]_D^{24}$ +39.9 (*c* 0.60, C_5H_5N), mp 264-266°C, and -6.4 (*c* 0.106, C_5H_5N), mp 250-252°C, respectively. Their HRFABMS suggested that the molecular formula was $C_{35}H_{55}O_8$ [M-H] (calcd. 603.3897, found 603.3953) for **1**, and $C_{35}H_{53}O_8$ [M-H] (calcd. 601.3791, found 601.3820) for **2**. The ^{13}C NMR spectra of **1** was very similar to that of hederagenin[2], and **2** to that of dodecandral[3] except the

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characteristic signals of D-xylose (**Table 1**), indicating **1** and **2** to be the glycosides of hederagenin and dodecandral with a pentose, respectively. And the obvious downfield shift for C-3 was observed for aglycone moiety: +8.5 ppm in **1**, +10.6 ppm for **2** (**Table 1**). Besides, the HMBC experiment showed the ^{1}H-^{13}C long-range connectivities for **1** between H-3 (δ 4.25) and C-1′ (δ 106.9), C-23 (δ 64.6), C-24 (δ 13.8); H-1′ (δ 5.02) and C-3 (δ 82.2), C-5′ (δ 67.2); for **2** between H-3 and C-1′ (δ 107.6), H-1′ and C-3 (δ 88.7), C-5′ (δ 67.1) (**Figure 1**).

Table 1 The NMR data of compound **1**, **2**, **3** and dodecandral (**4**)[a] in C_5D_5N

	1		**2**		**3**	**4**[3]
position	^{1}H[b]	^{13}C	^{1}H[b]	^{13}C	^{13}C	^{13}C
1	1.04, 1.55m	39.0	1.64 (m, 2H)	38.0	38.9	39.0
2	1.98, 2.22m	26.4	2.16 (m, 2H)	26.8	27.6	28.2
3	4.25 (dd, 4.5, 11.2)	82.2	3.34 (dd, 4.0, 11.9)	88.7	73.7	78.1
4	/	43.6	/	39.0	42.9	39.4
5	1.68m	47.7	0.83 (d, 7.5)	56.2	48.8	55.6
6	1.01, 1.06m	18.3	1.62 (m, 2H)	18.5	18.7	18.8
7	1.23 (m, 2H)	33.2	1.46 (m, 2H)	33.2	33.6	33.3
8	/	39.9	/	38.6	39.8	39.8
9	1.78m	48.3	1.66m	48.1	48.2	48.2
10	/	37.1	/	37.1	37.3	37.4
11	1.93, 2.05m	23.8	1.88 (m, 2H)	23.8	23.8	23.7
12	5.46br.s	122.7	5.53 br.s	123.5	122.7	122.4
13	/	145.0	/	144.2	145.0	144.6
14	/	42.3	/	42.1	42.2	42.2
15	1.11, 2.10m	28.5	2.16 (m, 2H)	28.3	28.4	28.4
16	1.16 (m, 2H)	24.1	2.10 (m, 2H)	23.6	23.8	23.8
17	/	46.8	/	46.3	46.7	46.3
18	3.25 (dd, 5.5, 14.2)	42.1	3.18 (dd, 3.6, 11.5)	43.1	42.0	43.2
19	1.30, 1.77m	46.8	2.07 (m, 2H)	40.2	46.5	40.4
20	/	31.1	/	46.9	31.0	46.9
21	1.18 (m, 2H)	34.5	1.98 (m, 2H)	28.1	34.3	28.2
22	1.76 (m, 2H)	33.4	1.87 (m, 2H)	33.8	33.3	33.9
23	3.69 (d, 10.7), 4.31 (d, 10.7)	64.6	1.29 (s, 3H)	28.3	68.2	28.8
24	0.93 (s, 3H)	13.8	0.98 (s, 3H)	17.0	13.1	16.6
25	0.94 (s, 3H)	16.3	0.80 (s, 3H)	16.5	16.0	15.6
26	1.00 (s, 3H)	17.6	0.96 (s, 3H)	17.3	17.5	17.5
27	1.27 (s, 3H)	26.4	1.30 (s, 3H)	26.4	26.2	26.4
28	/	180.4	/	180.1	180.4	180.3
29	0.92 (s, 3H)	33.5	0.94 (s, 3H)	24.1	33.3	24.2
30	0.99 (s, 3H)	24.0	9.63s	206.2	23.8	206.4
1′	5.02 (d, 7.5)	106.9	4.84 (d, 7.5)	107.6	/	/
2′	3.99 (dd, 7.5, 8.5)	75.7	4.03 (t, 8.3)	76.0	/	/
3′	4.06 (dd, 7.5, 8.5)	78.7	4.19 (dd, 8.3)	78.6	/	/
4′	4.18 (ddd, 4.2, 8.5, 8.5)	71.3	4.24 (ddd, 4.2, 8.0, 8.3)	71.2	/	/
5′	3.64 (dd, 4.2, 11.1), 4.29 (dd, 8.5, 11.1)	67.2	3.80 (dd, 4.2, 11.0), 4.00 (dd, 8.0, 11.0)	67.1	/	/

[a] ^{1}H, ^{13}C NMR and HMBC spectra were obtained at 500 MHz, 125 MHz and 500 MHz.
[b] Coupling constants are presented in Hz.
Unless otherwise indicated, all proton signals integrate to 1 H.

Acidic hydrolysis of **1** with 10% HCl gave hederagenin (**3**) and D-xylose, and **2** gave dodecandral (**4**) and D-xylose, which were identified by TLC comparing with authentic samples and EIMS method. Thus, the structures of **1** and **2** were elucidated as hederagenin-3-*O*-β-D-xylopyranoside, and dodecandral-3-*O*-β-D-xylopyranoside, respectively.

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Received 27 June, 2001