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Saikosaponin v-2 from *Bupleurum chinense*

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Abstract: Saikosaponin v-2(**1**), was isolated from the roots of the title plant and the structure was identified on the basis of spectral analysis. Saikosaponin v-2 is a new compound, which was identified as 3β,16α,23,28-tetrahydroxy-olean-11,13(18)-dien-30-oic acid-3-O-β-D-glucopyranosyl-(1→2)glucopyranosyl-(1→3)-β-D-fucopyranosyl-30-O-xylitol ester.

Keywards: *Bupleurum chinense* DC., *Umbelliferae*, saikosaponin v-2.

Bupleurum chinense DC. is a well-known and very important traditional chinese drug. It is often used to treat common cold with fever, alternating chill and fever, the feeling of fullness and oppression in the chest. However, little is reported about the chemical constituents. We have reported the isolation and elucidation of saponins and other compounds from the roots of *Bupleurum chinense* DC[1]. This paper deals with the structure elucidation of the new compound, Saikosaponin v-2(**1**).

Saikosaponin v-2 (**1**), white powder, mp 238-243°C, showed positive to both Molish and Liebermann-Burchard reactions. The UV spectrum showed absorption bands at 242, 251 and 261 nm, he ^{1}H NMR spectrum exhibited five angular methyl signals (δ 0.81, 0.97, 1.01, 1.44 and 1.62), two signals at 6.57 (1H, d, J = 10.5Hz, H-11) and 5.65 (1H, d, J = 10.5Hz, H-12), the ^{13}C NMR spectrum exhibited four signals at 137.5, 130.8, 127.0 and 125.9 corresponding to C-13, 18, 12 and 11, respectively. These data indicated that **1** had the skeleton of olean-11,13 (18) -diene. The ^{13}C NMR spectrum of **1** showed that the aglycone moiety possessed four hydroxyl groups at δ 82.0, 67.5 (CHOH) and at δ 64.1, 64.8 (CH_2OH), one xylitol group and a carbonyl group at δ 178.9, and the ^{13}C NMR data of the aglycone moiety were in good agreement with those of saikosaponin v-1 (**2**)[2]. Therefore, the structure of aglycone was identified as 3β, 16α, 23,28-tetrahydroxy-olean-11,13 (18)-dien-30-oic acid-30-O-xylitol ester. Acidic hydrolysis of **1** on TLC gave fucose and glucose which were identical with authentic samples. The signals at δ 5.08 (1H, d, J = 8.0Hz), 4.99 (1H, d, J = 8.0Hz), 4.97 (1H, d, J = 8.0Hz) , 1.43 (3H, d, J = 6.2Hz) in the ^{1}H NMR and δ 107.1, 105.3, 104.6, 17.2 in the ^{13}C NMR spectrum (**Table 1**) indicated that **1** was a triglycoside containing one fucose and two glucoses with β-anomeric configuration. So there is one more glucose in **1** than in **2**.

A comparison of the ^{13}C NMR data of **1** with those of saikosaponin v-1 (**2**) showed that the signal for C-2 of glucose in **1** was downfield shifted for 10.8 ppm and had 6 more signals for a second glucose than **2**. These results indicated that three sugars were linked to the genin *via* the C-3 hydroxy group and there was a 1→2 linkage between the

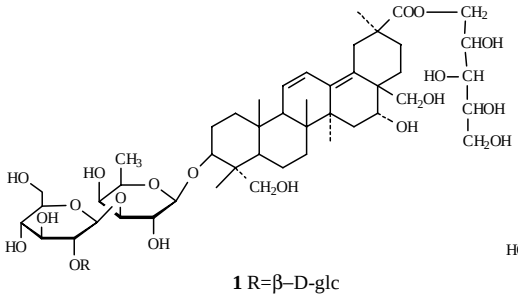
two glucoses. In the ^{13}C NMR spectrum, the signals for the three sugars of **1** were in good agreement with those of 2″-O-β-D-glucopyranosyl-saikosaponin b_2 (**3**), A quasi-molecular ion was observed at *m/z* 1129$[M+Na]^+$ and 1145$[M+K]^+$ in the TOF-MS.

Thus **1** was elucidated as 3β,16α,23,28-tetrahydroxy-olean-11,13 (18)-diene-30-oic acid-3-O-β-D-glucopyranosyl-(1→2)-β-D-glucopyranosyl-(1→3)-β-D-fucopyranosyl-30 -O-xylitol ester. **1** was a new saponin named saikosaponin v-2.

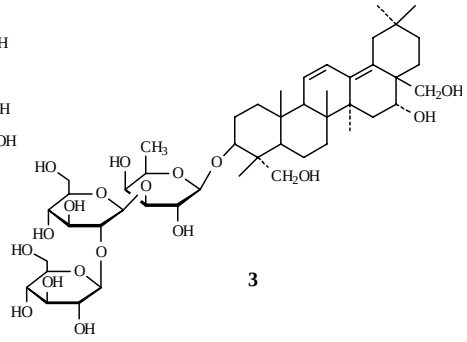
Table 1 ^{13}C NMR spectra data of compounds **1-3** (125MHz, C_5D_5N)

C	1	2	C	1	2	C	1	2	3
1	38.3	38.3	19	31.7	31.7	Fuc 1	105.3	105.9	105.4
2	26.1	26.1	20	44.2	44.2	2	71.1	71.8	71.3
3	82.0	81.6	21	30.7	30.7	3	86.7	85.2	86.9
4	43.6	43.6	22	23.7	23.7	4	71.7	72.2	71.8
5	47.3	47.3	23	64.1	64.0	5	70.8	71.0	71.0
6	18.1	18.1	24	13.0	13.1	6	17.2	17.2	17.4
7	32.2	32.2	25	18.8	18.8	Glc 1	104.6	106.6	104.8
8	41.0	41.0	26	17.1	17.2	2	86.0	75.8	86.2
9	53.9	53.9	27	21.7	21.7	3	77.7	78.4	77.8
10	36.4	36.4	28	64.8	64.8	4	70.8	71.5	71.0
11	127.0	126.8	29	21.0	20.9	5	78.4	78.7	78.5
12	125.9	125.9	30	178.5	178.9	6	62.0	62.6	62.1
13	137.5	137.5	Xylitol 1	67.5	67.5	Glc 1	107.1		107.2
14	41.9	41.9	2	72.2	72.2	2	76.5		76.6
15	33.4	33.4	3	74.1	74.0	3	77.6		77.8
16	67.5	67.5	4	74.3	74.3	4	70.5		70.7
17	45.3	45.3	5	64.3	64.0	5	79.1		79.2
18	130.8	130.6				6	62.2		62.4

Figure 1 Structures of compounds **1-3**



1 R=β–D-glc
2 R=H



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