

## A New Ecdysteroid from *Rhaponticum uniflorum*

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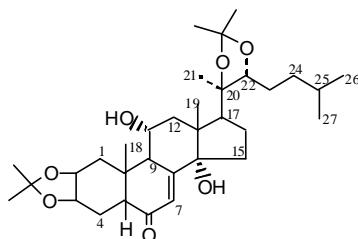
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**Abstract:** A new phytoecdysteroid was isolated from the root of *Rhaponticum uniflorum*. Its structure has been shown to be 2, 3, 20, 22-diacetonide ajugasterone.

**Keywords:** *Rhaponticum uniflorum*, compositae, 2, 3, 20, 22-diacetonide ajugasterone.

The root of *Rhaponticum uniflorum* (L.) DC. was used in China as a chinese traditional medicine for the treatment of fever and intoxications<sup>1</sup>. Since the 1980s this plant have been studied and some phytoecdysteroids and other compounds were isolated<sup>2-4</sup>. We report here the isolation and structural elucidation of a new ecdysteroid 2, 3, 20, 22-diacetonide ajugasterone (**1**), as well as the isolation of three known ecdysteroids, ecdysterone (**2**), ajugasterone C (**3**), ajugasterone C-20, 22-monoacetonide (**4**), from the roots of *R. uniflorum*.

**Figure 1** Structure of compound **1**



Compound **1** was isolated as white needles, mp 134-136°C,  $[\alpha]_D^{20} +58.2$  (c 1.0, MeOH). It has a molecular formula  $C_{33}H_{52}O_7$  based on FAB-MS ( $m/z$  560  $[M]^+$ ) and NMR spectral data. The IR spectrum of compound **1** contained absorption bands of hydroxy groups ( $3431\text{ cm}^{-1}$ ) and a keto group conjugated with a double bond ( $1662\text{ cm}^{-1}$ ).

Its UV spectrum ( $\lambda_{\text{max}}^{\text{MeOH}} 243\text{ nm}$ ) also confirmed the presence of a 7-en-6-keto group in the steroid nucleus. In the EI mass spectrum the peaks at  $m/z$  379, 361, 343 confirmed the existence of an ajugasterone C ring skeleton<sup>5</sup>. A strong peak at  $m/z$  185 could be the result of the side chain ion derived from cleavage between C-17 and C-20. The <sup>13</sup>CNMR spectrum (**Table 1**) showed that the compound is quite similar to ajugasterone C (**3**)

except that six more peaks corresponding to the ketal groups were observed ( $\delta$  108.09, 106.81, 26.76, 26.83, 29.04 and 30.87), and the C-2, C-3, C-20, C-22 signals shifted to down field. The mass spectrum of compound **1** showed the molecular ion peak at  $m/z$  560. This is 80 m.u. higher than the molecular weight of ajugasterone **3**. Accordingly, the structure of compound **1** is 2, 3, 20, 22-diacetonide ajugasterone.

Since no acetone was used in the extraction and subsequent treatment of the extractive substances, 2, 3, 20, 22-diacetonide ajugasterone (**1**) is a natural compound.

**Table 1** NMR assignment of compound **1** (in  $\text{CDCl}_3$ )

	$^{13}\text{C}$	$^1\text{H}$		$^{13}\text{C}$	$^1\text{H}$
1	39.98 t	1.44 m, 2.56 m	18	17.70 q	0.78 s
2	72.64 d	4.52 m	19	23.59 q	1.04 s
3	71.59 d	4.29 m	20	83.90 s	
4	36.35 t	1.74 m, 1.87 m	21	21.84 q	1.16 s
5	52.09 d	2.23 m	22	81.57 d	3.60
6	203.29 s		23	27.12 t	1.37 m, 1.54 m
7	122.13 d	5.85	24	36.38 t	1.25 m, 1.54 m
8	161.14 s		25	28.22 d	1.58
9	41.88 d	2.84	26	22.45 q	0.89 d (6.5)
10	38.58 s		27	22.58 q	0.91 d (6.5)
11	68.09 d	4.12 m	ketal group		
12	42.39 t	2.12 m, 2.23 m	-O-C-O-	108.09 s	
13	47.14 s			106.81 s	
14	84.42 s		$\text{CH}_3$	26.76 q	1.32 s
15	31.65 t	1.74 m, 2.10 m	$\text{CH}_3$	26.83 q	1.41 s
16	21.16 t	2.04 m, 2.13 m	$\text{CH}_3$	29.04 q	1.33 s
17	48.79 d	2.21	$\text{CH}_3$	30.87 q	1.49 s

\*J (Hz) in parentheses

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