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A New Ecdysteroid from *Rhaponticum uniflorum*

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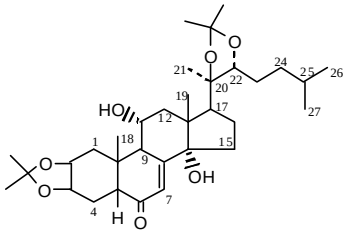
Abstract: A new phytoecdysteroid was isolated from the root of *Rhaponticum uniflorum.* Its structure has been shown to be 2, 3, 20, 22-diacetonide ajugasterone.

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[1]. Since the 1980s this plant have been studied and some phytoecdysteroids and other compounds were isolated[2-4]. 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 cm^{-1}) and a keto group conjugated with a double bond (1662 cm^{-1}). Its UV spectrum (λ_{max}^{MeOH} 243 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[5]. 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 ^{13}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 (δ 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 C **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 $CDCl_3$)

	^{13}C	$^{1}H^{*}$		^{13}C	^{1}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		CH_3	26.76 q	1.32 s
15	31.65 t	1.74 m, 2.10 m	CH_3	26.83 q	1.41 s
16	21.16 t	2.04 m, 2.13 m	CH_3	29.04 q	1.33 s
17	48.79 d	2.21	CH_3	30.87 q	1.49 s

*J (Hz) in parentheses

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