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New Diterpenoid Alkaloids from the Roots of *Aconitum excelsum* Reichb

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Abstract: Two new diterpenoid alkaloids have been isolated from roots of Aconitum excelsum Reichb. These new compounds were named excecoitine **I** and exceconidine **II**. The two structures were elucidated by spectroscopic methods as well as comparison with known compounds.

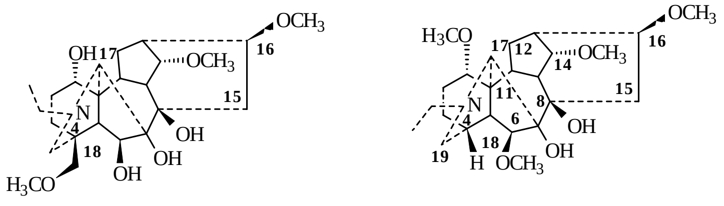
Keywords: Diterpenoid alkloids, exceconitine, exceconidine.

The plant Aconitum excelsum reichb native to China was collected in northeast Inner Monglia. The whole herb is used in Mongolian medicine for chronic bronchitis[1]. In the course of the investigation on the roots, we isolated two new and seven known diterpenoid alkaloids. Here we report the account on the structures of two new diterpenoid alkaloids.

Exceconitine **I**, colorless crystals, mp 202-204°C. The formula was determined as $C_{24}H_{39}O_7N$ on the basis of EIMS spectrum, m/z 453 (M^+,60) in combination with proton and carbon counts from NMR spectra. ^{1}HNMR spectrum exhibited three signals for the protons of three methoxy groups at δ 3.35, 3.36 and 3.40 (each 3H, s) and one N-ethyl with a triply MC signialt at δ1.12. Thus, the expanded formula is $C_{19}H_{21}$ (3x OCH_3+NCH_2CH_3+4x OH). Twenty-four signals in ^{13}CNMR (DEPT **Table 1**) were recognized (4x CH_3, 7x CH_2, 9x CH, 4x C). One of the methoxy groups at δ 59.5 was assigned to C-18 since the chemical shift of methene at C-18 (δ 78.8) approaches 77.3 as the case of delsoline[2a]. The other methoxy groups at δ 57.6 and 56.2 ppm were located at C-14 and C-16 by biogenetic cosideration and comparison with delsoline[2a]. One hydroxy group was located at C-1 (δ 72.5) by comparing the chemical shift C-19 (δ 57.8)[3] as well as the abundance of the molecular ion peak at m/z 453 in EIMS. Three other hydroxyl groups were assigned to C-6, C-7 and C-8 (δ 80.6, 87.9, 79.2) by comparing with acosanine[2b]. The above mentioned spectral data enabled us to propose the structure of **I** shown in **Figure**.

Exceconidine **II** was isolated as white power. The formula was determined as $C_{24}H_{39}O_6N$ on the basis of EIMS spectrum, m/z 437 (M^+, 10), in combination with proton and carbon and carbon counts from NMR spectra. ^{1}HNMR spectrum exhibited four signals for the protons of four methoxy groups at δ 3.24, 3.32, 3.37 and 3.40 (each 3H, s) and one N-ethyl at δ 1.04. Thus, the expanded formula is $C_{18}H_{19}$ (4x OMe+ NCH_2CH_3+2X OH). Twenty-four signals in ^{13}CNMR (DEPT **Table 1**) were recognized (5x CH_3, 6x CH_2, 10x CH, 3x C). The absence of methene signal at δ 65-90 in ^{13}CNMR (DEPT) indicated that **II** was a C_{18}-diterpenoid alkaloid. The methoxy groups at δ 56.0, 58.3 and 56.2 ppm were assigned to C-1, C-14 and C-16 by comparing with lycoctonine 2c and biogenetic consideratioon. By comparing the ^{13}CNMR data with umbofine **4**, two signals for quaternary carbons at δ 88.6 and 77.7 ppm could be tentatively assigned to C-7 and C-8 with hydroxyl groups. The special methenyl signal at δ 94.5 was assigned to C-6 with methoxy group. Consequently, the struture of **II** was as that illustrated in the **Figure**.

Figure.



I **II**

Table 1. ^{13}CNMR data of **I.II**

C	I	II	C	I	II
1	72.5d	84.9d	14	84.7d	83.9d
2	29.1t	26.0t	15	36.3t	33.4t
3	30.6t	29.4t	16	82.6d	82.8d
4	37.5s	38.3d	17	66.8d	65.1d
5	43.9d	43.4d	18	78.8t	--
6	80.6d	94.4d	19	57.8t	51.2t
7	87.9s	88.6s	N-CH2	50.5t	50.2t
8	79.2s	77.7s	-CH3	13.6q	14.1q
9	49.0d	48.7d	C-1'	--	56.0q
10	36.9d	36.8d	C-6'	--	57.7q
11	49.0s	48.7s	C-14'	57.6q	58.3q
12	27.4t	29.0t	C-16'	56.2q	56.2q
13	43.4d	46.2d	C-18'	59.5q	--

* s.d.t and q refer to C. CH. CH2. CH3. In DEPT respectively.

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