SUPPLEMENTARY MATERIAL

A New C₂₀-diterpenoid Alkaloid from the Lateral Roots of *Aconitum carmichaeli*

Jing Yu¹, Tian-Peng Yin¹, Jia-Peng Wang, Rui-Feng Mei, Le Cai* and
Zhong-Tao Ding*

School of Chemical Science and Technology, Yunnan University, Kunming, PR China

caile@ynu.edu.cn; ztding@ynu.edu.cn

Abstract

A new C₂₀-diterpenoid alkaloid carmichaedine (**1**) and six known alkaloids (**2-7**) were isolated from the lateral roots of *Aconitum carmichaeli*. Their structures were established on the basis of extensive spectroscopic analyses. Compound **1** exhibited potent antibacterial activity against *Bacillus subtilis* with minimum inhibitory concentration of 8 µg/mL.

Keywords: *Aconitum carmichaeli*; Ranunculaceae; diterpenoid alkaloid; carmichaedine, antibacterial

Figure S1. Key ^1H - ^1H COSY (—), HMBC ($\curvearrowright$) and NOESY ($\cdots$) correlations of compound **1**.

Figure S2. MS spectra of compound **1**.

Elemental composition calculator

Target m/z: +572.3218 amu
Tolerance: +100.0000 ppm
Result type: Elemental
Max num of results: 100
Min DBE: -0.5000 Max DBE: +50.0000
Electron state: Even
Num of charges: 1
Add water: N/A
Add proton: N/A
File Name: NJ-94+.wiff

	Elements	Min Number	Max Number
1	Br	0	0
2	C	0	32
3	F	0	0
4	H	0	46
5	Ir	0	0
6	N	0	1
7	Na	0	0
8	O	0	8
9	S	0	0

	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C32 H46 N O8	572.3217	0.0056	0.0098	10.5

Figure S3. ^1H NMR spectra of compound **1**.

Figure S4. ^{13}C NMR spectra of compound **1**.

Figure S5. ^1H - ^1H COSY spectra of compound **1**.

Figure S6. NOESY spectra of compound **1**.

Figure S7. HMQC spectra of compound **1**.

Figure S8. HMBC spectra of compound **1**.