SUPPLEMENTARY MATERIAL

A New C₂₀-Diterpenoid Alkaloid from *Aconitum soongaricum* var. *pubescens*

Lin Chen^{a,b,c}, Lianhai Shan^a, Wenliang Xu^a, Jifa Zhang^a, Shuai Huang^{a*} and Xianli Zhou^{a,b*}

^a*School of Life Science and Engineering, Southwest Jiaotong University, Chengdu, 610031 China*

^b*Key Laboratory of Advanced Technologies of Materials, Ministry of Education, School of Material Science and Engineering, Southwest Jiaotong University, Chengdu, 610031 China*

^c*School of Chemistry and Chemical Engineering, China West Normal University, Nanchong, 637002 China*

Corresponding authors:

1. Dr. Shuai Huang; Phone: +86-28-87600951; Email: shuaih@home.swjtu.edu.cn;
2. Dr. Xianli Zhou; Phone: +86-28-887603201; Email: xxbiochem@163.com.

ABSTRACT

A new denudatine-type C₂₀-diterpenoid alkaloid, pubesine (**1**), along with seven known diterpenoid alkaloids, altaconitine (**2**), 14-benzoylaconine (**3**), spicatine A (**4**), 14-benzoylaconine-8-palmitate (**5**), 14-O-acetylsenbusine A (**6**), senbusine A (**7**) and 14-acetylneoline (**8**) were isolated from the whole plant of *Aconitum soongaricum* var. *pubescens*. Their structures were elucidated by means of extensive spectroscopic analyses (NMR and HR-ESI-MS) and comparison with data reported in the literature. All compounds were evaluated for their cytotoxicity against H460, MCF-7 and Hep G2 human cancer cell lines.

Keywords: Diterpenoid alkaloid; Pubesine; *Aconitum Soongaricum* var. *pubescens*; Cytotoxic activity

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Figure S1. IR spectrum for compound **1**

Figure S2. HR-ESI-MS spectrum for compound **1**

Elemental Composition Report

Elements Used: C: 0-100 H: 0-200 N: 0-10 O: 0-20

Minimum:	80.00			-1.5				
Maximum:	100.00	5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
402.2279	402.2280	-0.1	-0.2	8.5	591.6	0.003	99.74	C23 H32 N O5
	402.2294	-1.5	-3.7	13.5	597.6	5.973	0.25	C24 H28 N5 O
	402.2254	2.5	6.2	9.5	601.0	9.395	0.01	C19 H28 N7 O3

Figure S3. ^1H NMR spectrum for compound **1**

Figure S4. ^{13}C NMR spectrum for compound **1**

Figure S5. DEPT ($\theta = 135^\circ$) spectrum for compound **1**

Figure S6. ^1H - ^1H COSY spectrum for compound **1**

Figure S7. HMQC spectrum for compound **1**

Figure S8. HMBC spectrum for compound **1**

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Figure S10. Key ^1H - ^1H COSY, HMBC and ROESY correlations of **1**.