SUPPLEMENTARY MATERIAL

A New isocoumarin from the Aerial Parts of *Aconitum gymnandrum*

Jian-Qiang Zhao^{ac#}, Yan-Ming Wang^{bc#}, Shuo Wang^a, Jun Dang^a, Yan-Ping Shi^b, Li-Juan Mei^{a*}, and Yan-Duo Tao^{a*}

^aKey Laboratory of Tibetan Medicine Research of CAS and Key Laboratory for Tibetan Medicine of Qinghai Province, Northwest Institute of Plateau Biology, Chinese Academy of Sciences, Xinning 810008, P. R. China

^bKey Laboratory of Chemistry of Northwestern Plant Resources of CAS and Key Laboratory for Natural Medicine of Gansu Province, Lanzhou Institute of Chemical Physics, Chinese Academy of Sciences, Lanzhou 730000, P. R. China

^cUniversity of Chinese Academy of Sciences, 100049, Beijing, P. R. China

[#]The authors contributed equally to this paper

A new isocoumarin, along with ten known compounds, was isolated from the aerial parts of *Aconitum gymnandrum*. Their structures were elucidated by spectroscopic methods including extensive 1D and 2D NMR techniques. Among the known compounds, compound **11** was obtained as a natural product for the first time, which was previously reported as a synthetic product. In addition, compounds **1–5**, **7** and **9** were tested for their cytotoxicity against four human cancer cell lines. The results showed that compounds **3**, **4** and **7** displayed cytotoxicity against lung cancer A549 and gastric cancer MGC80, respectively, whereas **5** and **9** showed selective cytotoxicity against hepatocellular carcinoma HepG2.

Keywords: *Aconitum gymnandrum*, isocoumarin, cytotoxic activity

* Corresponding author. Phone: +86-971-6143610, fax: +86-971-6143610. e-mail: meilijuan111@163.com (L.-J. Mei), tyd@nwipb.cas.cn (Y.-D. Tao).

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Table S1. ^1H and ^{13}C NMR Spectroscopic Data of Compounds **1** (600 and 150 MHz, resp.; δ in ppm, CD_3OD)

position	δ_{H} (mult. J in Hz)	δ_{C}
1		171.8, C
3	4.47, dt (13.0, 8.3)	80.3, CH
4	2.82, m	33.6, CH_2
5	6.28, s	107.9, CH
6		158.4, C
7		135.2, C
8		157.6, C
9		102.3, C
10		137.5, C
α	2.08, m	37.8, CH_2
	1.97, m	
β	2.81, m	31.2, CH_2
	2.73, ddd (13.9, 9.3, 7.1)	
1'		134.4, C
2', 6'	7.14, d (8.7)	130.5, CH
3', 5'	6.83, d (8.7)	115.1, CH
4'		159.7, C
6-MeO	3.75, s	55.8, CH_3
7-MeO	3.82, s	61.0, CH_3

Figure S1. Critical HMBC (H $\rightarrow$ C) and ^1H - ^1H COSY (H $\longleftrightarrow$ H) correlations of compound **1**.

Figure S2 ^1H NMR spectrum of 6,7-dimethoxy-8-hydroxy-3- $[\beta$ -(*p*-hydroxyphenyl)ethyl]-3,4-dihydroisocoumarin (**1**)

yumf-14-4-2-H

STANDARD PROTON PARAMETERS

Figure S3 ^{13}C NMR spectrum of 6,7-dimethoxy-8-hydroxy-3- $[\beta$ -(*p*-hydroxyphenyl)ethyl]-3,4-dihydroisocoumarin (**1**)

yumf-14-4-2-C
STANDARD CARBON PARAMETERS

Figure S4 HSQC spectrum of 6,7-dimethoxy-8-hydroxy-3- $[\beta$ -(*p*-hydroxyphenyl)ethyl]-3,4-dihydroisocoumarin (**1**)

Figure S5 HMBC spectrum of 6,7-dimethoxy-8-hydroxy-3- $[\beta$ -(*p*-hydroxyphenyl)ethyl]-3,4-dihydroisocoumarin (**1**)

Figure S6 COSY spectrum of 6,7-dimethoxy-8-hydroxy-3-[β -(*p*-hydroxyphenyl)ethyl]-3,4-dihydroisocoumarin (**1**)

Figure S7 HR-ESI-MS of 6,7-dimethoxy-8-hydroxy-3- $[\beta$ -(*p*-hydroxyphenyl)ethyl]-3,4-dihydroisocoumarin (**1**)

zhaojianqiang-5_150604151618

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Y14-4-2

.9 ppm

NL:
1.91E6
zhaojianqiang-
5_150604151618#16
RT: 0.11 AV: 1 T:
FTMS + p ESI Full ms
[115.00-2000.00]

NL:
8.01E5
C₁₉H₂₀O₆ +H:
C₁₉H₂₁O₆
pa Chrg 1