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A New Iridoid Glucoside from *Lagotis yunnanensis*

Xiao Dong YANG[1], Shuang Xi MEI[1, 2], Jing Feng ZHAO[1], Gan Peng LI[1, 3], Hong Bin ZHANG[1], Liang LI[1]*

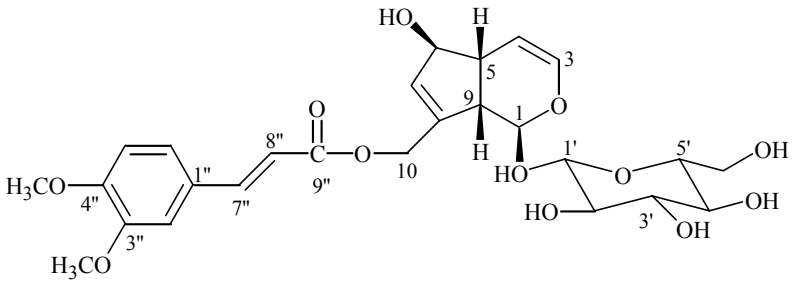
[1]School of Pharmacy, Yunnan University, Kunming 650091
[2]School of Life Science, Yunnan University, Kunming 650091
[3]Department of Chemistry, Lanzhou University, Lanzhou 730000

Abstract: Phytochemical investigation of *Lagotis yunnanensis* led to the isolation and identification of a new iridoid glucoside **1**, named as 10-*O*-(3, 4-dimethoxy-(*E*)-cinnamoyl)aucubin. Its structure was elucidated by spectroscopic methods.

Keywords: *Lagotis yunnanensis*, iridoid glucoside, 10-*O*-(3, 4-dimethoxy-(*E*)-cinnamoyl)aucubin.

Lagotis yunnanensis W. W. Smith is distributed in the southwest of China. It is used in Tibetan folk medicine for treatment of fever, hypertension, and acute and chronic hepatitis[1]. To the best of our knowledge, no phytochemical study on *Lagotis yunnanensis* has been reported. Eight kilograms dried aerial part of the titled plant collected in the northwest of Yunnan Province were investigated by us. As a result, a new compound (**1**) and several known iridoid glucosides were isolated. Compound **1** was identified as 10-*O*-(3, 4-dimethoxy-(*E*)-cinnamoyl)aucubin.

Figure 1 The structure of **1**



Compound **1** was isolated as a white amorphous powder, $[\alpha]_D^{24}$ –60.07 (*c* 0.283, CH_3OH). Its molecular formula was determined as $C_{26}H_{32}O_{12}$ by HREIMS (found 536.1940, calcd. 536.1894). The IR spectrum showed characteristic absorptions for OH (3448 cm^{-1}, br), *α*, *β*-unsaturated ester (1700 and 1630 cm^{-1}), and aromatic-ring (1598

* E-mail: liliang5758@sina.com

Figure 2 The key correlations in HMBC and NOESY spectrum of **1**

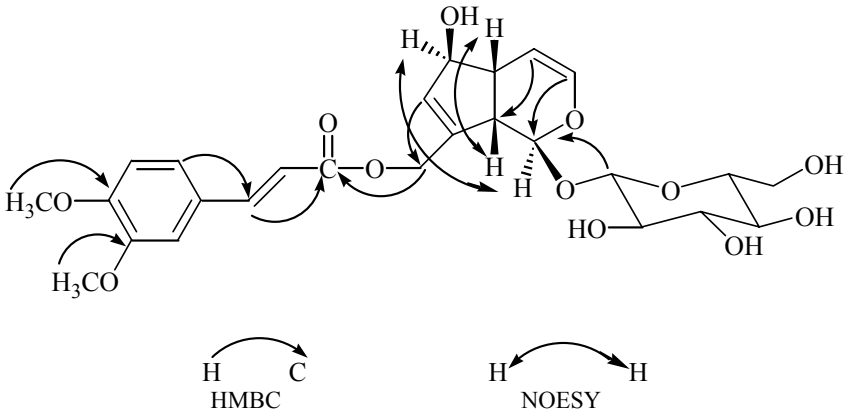


Table 1 ^{1}H (500 MHz) and ^{13}C NMR (125 MHz) data of **1** in DMSO-d_6, (δ in ppm)

C	δ_C	δ_H (*J*, Hz)	C	δ_C	δ_H (*J*, Hz)
1	95.71 (d)	4.87 (d, 1H, 7.4)	6′	61.08 (t)	
3	140.25 (d)	6.37 (dd, 1H, 6.0, 2.0)	6′a		3.65 (d, 1H, 11.9)
4	104.61 (d)	5.06 (dd, 1H, 6.0, 3.8)	6′b		3.60 (m, 1H)
5	44.58 (d)	2.58 (m, 1H)	1″	126.75 (s)	
6	80.50 (d)	4.37 (br, s, 1H)	2″	111.53 (d)	7.35 (d, 1H, 1.9)
7	132.35 (d)	5.81 (br, s, 1H)	3″	144.92 (s)	
8	139.78 (s)		4″	151.00 (s)	
9	46.53 (d)	2.85 (dd, 1H, 7.4, 7.9)	5″	110.36 (d)	7.00 (d, 1H, 8.0)
10	61.70 (t)	4.82 (s, 2H)	6″	122.94 (d)	7.26 (dd, 1H, 8.0, 1.9)
1′	98.27 (d)	4.56 (d, 1H, 7.5)	7″	148.93 (d)	7.64 (d, 1H, 15.9)
2′	73.27 (d)	3.14 (dd, 1H, 9.1, 7.5)	8″	115.24 (d)	6.60 (d, 1H, 15.9)
3′	76.50 (d)	3.42 (dd, 1H, 9.1, 8.7)	9″	166.16 (s)	
4′	70.00 (d)	3.20 (m, 1H)	OCH_3	55.57 (q)	3.82 (s, 3H)
5′	77.00 (d)	3.19 (m, 1H)		55.53 (q)	3.81 (s, 3H)

and 1510 cm^{-1}). The UV absorption at 234, 296 and 322 nm also confirmed the existence of these unsaturated functional groups. From its NMR spectrum (**Table 1**), the signals of a *β-D*-glucose ($C_{1'}$-$C_{6'}$, $H_{1'}$-$H_{6'}$) and a 3, 4-disubstituted-(*E*)-cinnamoyl ($C_{1''}$-$C_{9''}$, $H_{2''}$, $H_{5''}$, $H_{6''}$, $H_{7''}$ and $H_{8''}$) were observed. ^{13}C and DEPT NMR experiments differentiated the skeleton carbons of **1** as 1×CH_2 (61.70, C-10), 7×CH [including three olefinic carbons (140.25, 104.61, and 132.35, corresponding to C-3, C-4, and C-7, respectively), one oxygenated methine (80.50, C-6), one hemiacetal (95.71, C-1), C-5 (44.58) and C-9 (46.53)], 1×C (139.78, C-8). The above spectral information indicated that compound **1** is an analogue of 10-*O*-((*E*)-cinnamoyl)aucubin[2]. In HMBC spectrum (**Figure 2**), the correlations of δ_H 4.56 (H-1′) to δ_C 95.71 (C-1) suggested that *β-D*-glucose was substituted at C-1 position, while δ_H 4.82 (H-10) to δ_C 166.16 (C-9″) indicated that 3, 4-disubstituted-(*E*)-cinnamoyl was substituted at C-10 position. The correlations between δ_H 3.81 (OCH_3) to δ_C 144.92 (C-3″) and δ_H 3.82 (OCH_3) to δ_C 151.00 (C-4″) suggested that the cinnamoyl is 3, 4-dimethoxy-(*E*)-cinnamoyl. NOESY experiments were also conducted and the key correlations are indicated in **Figure 2**.

The correlations between H-1 and H-6 as well as H-5 and H-9 suggested that the relative configuration of C-1, C-6, C-5 and C-9 in compound **1** are similar to that of 10-*O*-((*E*)-cinnamoyl)aucubin. Therefore, compound **1** was elucidated as 10-*O*-(3, 4-dimethoxy-(*E*)-cinnamoyl)aucubin.

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