Chinese Chemical Letters Vol. 12, No. 4, pp. 343 – 344, 2001

A New Monoterpene Glucoside from the Leaves of *Betula platyphylla* Suk.

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Abstract: A new monoterpene glucoside, (2E,6Z)-2,6-dimethyl-8-β-D-glucosyloxy-2,6-octadien-oic acid, was isolated from the leaves of *Betula platyphylla* Suk. The structure was established by spectroscopic data.

Keywords: *Betula platyphylla* Suk., monoterpene glucoside, leaves.

Betula platyphylla Suk., whose bark and juice are used as anti-inflammatory and cough relieving agent[1], is widespread in China. Previous investigations of this plant have led to the isolation of various compounds[2,3]. We herein report structural elucidation of a new monoterpene glucoside (**1**) isolated from the leaves of *Betula platyphylla* Suk.. Only two monoterpene glucosides isolated from *Betula* L. have been published until now[4].

Compound **1** was obtained as colorless needles (EtOAc), mp 64.5~66ºC. It showed positive bromocresol green reaction, which suggested a carboxyl group presented in **1**. Acidic hydrolysis of **1** on TLC gave D-glucose by comparison with authentic sample. The EIMS gave ion peaks at *m/z* 184 $[M-162]^+$, 166 $[M-180]^+$, which indicated the molecular formula of **1** as $C_{16}H_{26}O_8$ in combination with the ^1H and ^{13}C NMR spectrum. The ^1H NMR spectrum showed two olefinic protons at δ 6.76 (1H,br.t, J = 6.8Hz) and 5.38 (1H, br.t, J = 6.4Hz) which were linked with two methylene, respectively. A series of signals between δ 4.30 and 3.11 were ascribed to the β-D-glucosyl group which was indicated by δ 4.28 (1H, d, J = 7.5Hz). Two methyl (δ 1.77 and 1.81) and three methylene were also observed.

Figure 1 The structure of compound **1**

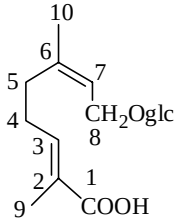
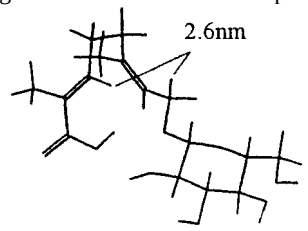


Figure 2 The gauche conformation of compound **1**



In ^{13}C NMR spectrum, ten carbon signals in addition to six glucosyl carbons between δ 102.8 and 62.9 were observed, which indicated **1** as monoterpene glucoside. The presence of α, β-unsaturated carbonyl was revealed by the resonance at δ 169.2, 142.3 (CH) and 128.7 (C). These results and the NOESY experiment suggested **1** as (2E, 6Z)-2,6-dimethyl-8-β-D-glucosyloxy-2,6-octadienoic acid. Interestingly, a weak cross peak was observed between H-3 and H-8, which revealed that some proportion of gauche conformation were existed in solution with a distance of 0.26 nm from H-3 to H-8 (calculated by Chem. 3D.).

Position	^{1}H NMR (δ)	^{13}C NMR (δ)	NOESY correlation
1	------	169.2	------
2	------	128.7	------
3	6.76 (1H,br.t,J=6.8Hz)	142.3	H-4, H-5, H-8
4	2.23 (2H,m)	31.3	H-3, H-9
5	2.20 (2H,m)	27.7	H-3, H-8, H-10
6	------	139.7	
7	5.38 (1H,br.t,J=6.4Hz)	123.5	H-8, H-10
8	4.30 (1H,dd,J=12.0,7.5Hz) 4.16 (1H,dd,J=12.0,6.4Hz)	65.3	H-3, H-7, H-5
9	1.77 (3H,s)	12.5	H-4
10	1.81 (3H,s)	23.4	H-7, H-5
1’	4.28 (1H,d,J=7.5Hz)	102.7	H-2’
2’	3.15 (1H,t,J=8.0Hz)	74.7	H-1’
3’	}	77.3	------
4’	3.34 (3H,m)	71.6	------
5’	}	77.9	------
6’	3.82 (1H,dd,J=11.7,2.5Hz) 3.63 (1H,dd,J=11.7,5.3Hz)	62.9	------

Table 1 ^{1}H, ^{13}C NMR data and NOESY correlation of **1**†

† ^{1}H &^{13}C NMR recorded on 300 &75 MHz in aceton-d_6 with chemical shifts (ppm) from TMS.

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Received 23 September, 2000