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A New Diterpene from *Suregada glomerulate(Blume)* Baill

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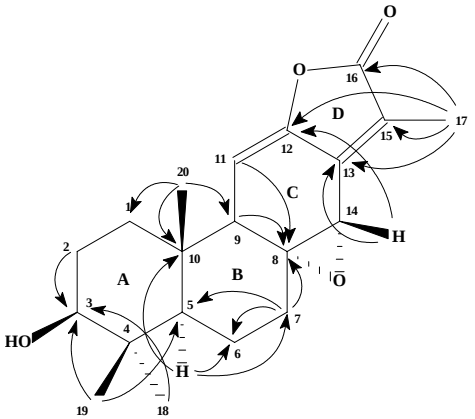
Abstract: A new diterpene with an abietane skeleton, 3*β*-hydroxy-8*α*,14*α*-epoxyabieta-11,13(15)-dien-16,12-olide, was isolated from the root of *Suregada glomerulate(Blume)* Baill. Its structure was elucidated on the basis of spectroscopic and X-ray crystallographic analysis.

Keywords: *Suregada glomerulate(Blume)* Baill, diterpene, abietane, 3*β*-hydroxy-8*α*,14*α*-epoxy-abieta-11,13 (15)-dien-16,12-olide, X-ray crystallographic analysis.

The genus suregada comprises about 40 species, which distribute in southeast of Asia and Oceania(north of Australia). *Suregada glomerulate(Blume)* Baill and *Suregada aequorea* are the only two species of this genus found in China[1]. *Suregada glomerulate (Blume)* Baill has not ever been reported for its chemical or medicinal research. A new diterpene with an abietane skeleton, 3*β*-hydroxy-8*α*,14*α*-epoxyabieta-11,13(15)-dien-16,12-olide, was obtained from the root of *Suregada glomerulate (Blume)* Baill. This paper deals with the structure elucidation of this compound.

Figure 1 The structure and key HMBC correlations of **1**



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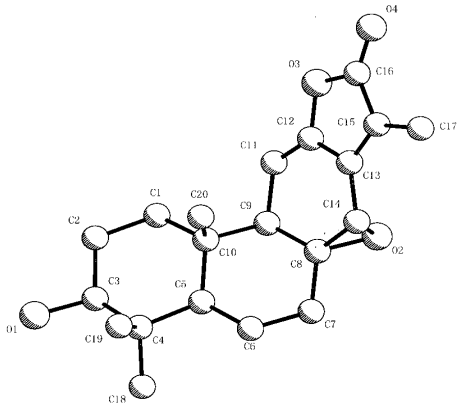
The EtOAc extract derived from the ethanolic extract was separated by silica gel column chromatographies to give the new compound, named 3*β*-hydroxy-8*α*,14*α*-epoxyabieta-11,13 (15)-dien-16,12-olide **1**.

Compound **1** was isolated as colorless needle, m. p. 247-248℃ (Me_2CO) , $[\alpha]_D^{25}$ +123 (*c* 0.10, $CHCl_3$). Its molecular formula was determined as $C_{20}H_{26}O_4$ by HREIMS *m/z* 330.1834 $[M]^+$(calcd. for $C_{20}H_{26}O_4$ 330.1831). IR spectrum (KBr) revealed the presence of hydroxyl (3579 cm^{-1}), *α*, *β* unsaturated *γ*-lactone carbonyl (1747 cm^{-1}) and olefinic groups (1653 cm^{-1}) in **1**. The NMR spectrum of **1** in $CDCl_3$ exhibited four methyl signals, two oxygen-substituted methines at δ_C 78.3 (C-3) and δ_H 3.72 (dd, 1H, *J* 4.5, 11.5Hz, H-3), δ_C 54.4 (C-14) and δ_H 3.72 (s, 1H, H-14), one carbonyl group of lactone (δ_C170.4) and four olefinic carbons. The ^1H and ^{13}C–NMR spectra of **1** were similar to those of *ent*-8*α*, 14*α*-epoxyabieta-11, 13 (15) -dien-16, 12-olide (jolkinolides A), except for A ring which has a substitution of 3*β*-OH[2]. This was confirmed by HMBC experiment (see **Figure 1**). The two methyl protons (*δ*1.08, H-18; *δ*0.84, H-19) as well as H-2 (*δ*1.69) showed long range correlations with C-3 (*δ*78.3) respectively which indicated that the hydroxy group might be located at C-3. The *β*-configuration of 3-hydroxy group was suggested by the large coupling constants between H-3 and H-2. ^1H and ^{13}C-NMR chemical shifts were assigned (see **Table 1**) from a combination of 2D heteronuclear ^{13}C-^1H (HMQC, HMBC) correlations. The relative configuration of **1** was comfirmed by X-ray crystallographic analysis, which indicated that an abietane skeleton for the molecule (see **Figure 2**).

Table 1 ^1H (500MHz) and ^{13}C (125MHz) NMR data of compound **1** in $CDCl_3$

No.	δ_H	δ_C (DEPT)
1	1.78(m,1H), 1.42(m,1H)	37.7(CH_2)
2	1.69(overlap,2H)	27.0(CH_2)
3	3.33(dd,1H,4.5,11.5)	78.3(CH)
4		39.2(C)
5	1.23(m,1H)	52.9(CH)
6	1.84(m,2H)	20.5(CH_2)
7	1.64(m,1H),2.11(m,1H)	34.0(CH_2)
8		61.0(C)
9	2.60(d,1H,5.0)	51.6(CH)
10		41.1(C)
11	5.42(d,1H,5.0)	103.4(CH)
12		147.7(C)
13		144.8(C)
14	3.72(s,1H)	54.4(CH)
15		125.5(C)
16		170.4(C)
17	2.06(s,3H)	8.7(CH_3)
18	1.08(s,3H)	28.3(CH_3)
19	0.84(s,3H)	15.6(CH_3)
20	0.74(s,3H)	15.0(CH_3)

Figure 2 The result of analysis X-ray structure of compounds **1**



Acknowledgment

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