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Two New Cycloartane Triterpenes from The Leaves of *Quercus valiabilis* Blume

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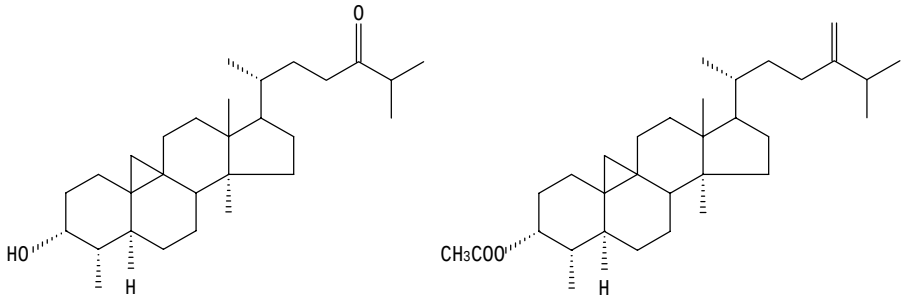
Abstract: Two new cycloartane triterpenes were separated from the leaves of *Quercus valiabilis* Blume. The structures were identified as 4α,14α-dimethyl-9β,19-cycloergost-3α-yl-24-one and 4α,14α-dimethyl-9β,19-cycloergost-24(24′)-en-3α-yl-acetate.

Keywords: *Quercus valiabilis* Blume, triterpene, cycloartane, cycloeucalenol.

The fruit of *Quercus valiabilis* Blume has been used as a kind of chinese traditional medicine. Our investigation on chloroform extract of the leaves of this plant resulted in the isolation of two new cycloartane triterpenes.

Figure 1 The structures of compound **1** and **2**



1 **2**

Compound **1** was obtained as colorless needles, and gave a positive Liebermann-Burchard test for triterpenoids. Its IR(KBr ν cm^{-1}) spectrum showed absorptions at 3431(hydroxy group), 1718(carbonyl group), 3040 and 1381(cyclopropyl group). The mass spectrum of compound **1** displayed $[M]^+$ at *m/z* 428 accompanied with diagnostic fragment ions peaks at *m/z* 300$[M\text{-}C_8H_{14}O(ringA)]^+$, 285$[M\text{-}C_8H_{14}O(ringA)\text{-}CH_3]^+$and

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175[M-$C_8H_{14}O$(ringA)-C_9H_{17}(side-chain)]$^+$, which were similar to those of cycloartane triterpenes. The ^{1}H NMR and ^{13}C NMR data of skeleton of compound **1** were quite similar to those of 3-epicycloeucalenol[1], and the side chain were similar to those of cycloartan-3,24-dione[2]. Thus, compound **1** was determined to be 4α,14α-dimethyl-9β,19-cycloergost-3α-yl-24-one [3-epicycloeucalenyl-24-one], which was confirmed by its DEPT, ^{1}H-^{1}H COSY, HMQC and HMBC spectra..

Table 1 ^{13}C NMR data of compound **1**, compound **2**

Carbon	compound **1**	Compound **2**
1	26.8	27.5
2	33.0	30.2
3	72.3	75.1
4	41.0	39.9
5	37.9	39.1
6	24.5	24.5
7	24.7	24.8
8	46.7	47.2
9	23.1	23.3
10	30.2	29.9
11	26.9	26.8
12	32.9	32.9
13	45.3	45.3
14	49.0	49.0
15	35.3	35.4
16	28.0	28.1
17	52.1	52.2
18	17.7	17.9
19	26.2	26.5
20	35.8	36.2
21	18.1	18.4
22	30.2	35.0
23	37.5	31.3
24	215.4	157.0
25	40.8	33.8
26	18.4	22.0
27	18.3	21.9
28	19.1	19.2
29	15.4	15.1
30	—	106.0
$OCOCH_3$	—	171.2
$OCOCH_3$	—	21.4

Compound **2** was also obtained as colorless needles, mp 88~90℃, and gave a positive Liebermann-Burchard test for triterpenoids. Its IR(KBr ν cm^{-1}) spectrum showed 1740 (carbonyl group), 1638 and 884 (terminal methylene group) and 3040, 974 (cyclopropyl group). The mass spectrum showed [M]$^+$ at *m/z* 468 accompanied with diagnostic fragment ions peaks at *m/z* 453[M-CH_3]$^+$, 408[M-CH_3COOH]$^+$, 300[M-$C_{10}H_{16}O_2$ (ringA)]$^+$, 285[M-$C_{10}H_{16}O_2$(ringA)-CH_3]$^+$ and 175[M-$C_{10}H_{16}O_2$(ringA)-C_9H_{17} (side- chain)]$^+$, which were similar to those of acetate of cycloartane triterpenes. ^{1}H NMR and ^{13}C NMR data of compound **2** were similar to those of 3-epicycloeucalenol except ring A. It showed a methine signal at δ 2.08 in the ^{1}H NMR spectrum and δ

21.4, 171.2 in the ^{13}C NMR spectrum, suggesting that it possessed an acetoxy group in ring A. From the above evidence, compound **2** was determined to be 3-epicyclo-eucalenyl-acetate[4α,14α-dimethyl-9β,19-cycloergost-24(24′)-en-3α-yl-acetate]. The structure was further confirmed by deacetylation.

References

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