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A new Kaurane Derivative from *Aralia Fargesii*

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Abstract: A new *ent*-kaurane diterpene was isolated from the rhizome of *Aralia fargesii.* On the basis of chemical and spectral evidences, its structure was established as 16α-hydroxy-17-isovaleroyloxy-*ent*-kauran-19-oic acid.

Keywords: *Aralia fargesii*, *ent*-kaurane, 16α-hydroxy-17-isovaleroyloxy-*ent*-kauran-19-oic acid.

As part of our chemical and chemotaxonomical studies of *Aralia* , we have investigated the chemical constituents of *Aralia fargesii,* which is one of the herbal plants of *Aralia*. This communication reports the structure elucidation of a new *ent*-kaurane derivative 16α- hydroxy-17-isovaleroyloxy-*ent*-kauran-19-oic acid **I** from *Aralia fargesii.* 3kg of plant *Aralia Fargesii* was extracted with petroleum ether and MeOH respectively, and the petroleum ether extract was rechromatographed resulting in the isolation of (22mg) 16α-hydroxy-17-isovaleroyloxy-*ent*-kauran-19-oic acid.

I was obtained as white needles (CH_3OH), mp 188-190℃, $[\alpha]_D^{20}$ -59 (c 0.1025, $CHCl_3$), with a molecular formula $C_{25}H_{40}O_5$, as supported by its HRFAB-MS (Found. 421.2974; Calcd. 421.2954), and the analysis of ^1H, ^{13}CNMR data. Its IR spectrum showed strong absorptions at 1740 and 1701 cm^{-1} owing to ester carbonyl and carboxyl groups respectively. The ^1HNMR spectrum (**Table 1**) showed two angular methyl signals (δ 0.93 and 1.22) and one doublet (J=6.5Hz) of dimethyl protons at δ 0.96 due to the isovaleroyloxy group. The ^{13}CNMR spectrum (**Table 2)** showed the presence of 25 carbon atoms. Two tertiary methyl resonances at δ 1.22 and 0.93 and the ^{13}CNMR resonances at δ 183.7(C-19), 28.9 (C-18) and 15.5 (C-20) were typical of the axial C-20 and equatorial C-18 in diterpenoids with a C-19 axial carboxyl acid[1]. The chemical shifts in the ^1H and ^{13}CNMR spectra of **I** were compared with those of 16α, 17-dihydroxy-*ent*-kauran-19 -oic acid[2] which gave very similar values except those for C-17 and those for isovaleroyloxy group. These results revealed that **I** had the 16α, 17-dihydroxy kauran-19-oic acid skeleton. The ^{13}CNMR spectra data of C-17 and isovaleroyloxy group of **I** were coincident with the known compound *ent*-16βH, 17-isovaleroyloxy-kauran-19-oic acid[1]. These indicated that **I** possessed the skeletal part of 16α, 17-dihydroxy-*ent*-kauran-19-oic acid and the sidechain part of *ent*-16βH, 17-isovaleroyloxy-kauran-19-oic acid. As a further supporting evidence,

the EI-MS of **I** exhibited a significant fragment peak at m/z 305 (basic peak), it is the fragment ion of (M^+-$CH_2OCOCH_2CH(CH_3)_2$). In the HMBC spectrum, the methylene signals at δ 4.20 (1H, d, J=11Hz) and δ 4.24 (1H , d , J=11Hz) were correlated to the carbon signal of ester carbonyl at δ 173.3 and suggested the isovalerate side chain must be attached to the C-17 hydrox methyl.

From these spectral data, the chemical structure of **I** was established as 16α-hydroxy-17-isovaleroyloxy-*ent*-kauran-19-oic acid.

Figure 1

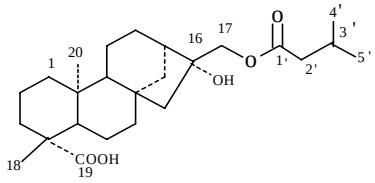

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Table 1. ^{1}HNMR spectral data of **I** （in $CDCl_3$,TMS as internal standard, 500 MHz）

No.	H		No.	H	
1	0.81	1.85	14	1.15	1.94
2	1.42	1.83	15	1.55	
3	1.03	2.13	17	4.20	4.24
5	1.04		18	1.22	
6	1.82	1.92	20	0.93	
7	1.43	1.64	2’	2.22	
9	0.99		3’	2.09	
11	1.49	1.59	4’	0.96	
12	1.46	1.57	5’	0.96	
13	2.03				

Table 2. ^{13}CNMR spectral data of **I** （in $CDCl_3$, 125MHz）

No	C	No	C	No	C
1	40.6	9	55.7	17	68.2
2	19.0	10	39.7	18	28.9
3	37.8	11	18.4	19	183.7
4	43.7	12	26.2	20	15.5
5	56.8	13	45.9	1’	173.3
6	22.0	14	37.0	2’	43.4
7	41.8	15	52.9	3’	25.8
8	44.8	16	80.2	4’	22.4
				5’	22.4

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