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Two New Pentacyclic Triterpenes from *Sabia parviflora*

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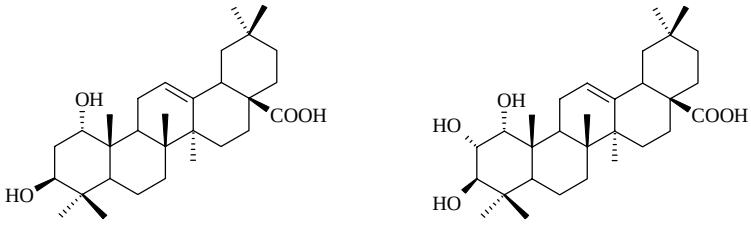
Abstract: Two new pentacyclic triterpene acids, 1α, 3β-dihydroxyl-olean-12-en-28-oic acid and 1α, 2α, 3β-trihydroxyl-olean-12-en-28-oic acid, were isolated from the arial parts of *Sabia parviflora*.

Keywords: *Sabia parviflora*, pentacyclic triterpene acid, 1 α, 3β-dihydroxyl-olean-12-en-28-oic acid , 1α, 2α, 3β-trihydroxyl-olean-12-en-28-oic acid.

Sabia parviflora Wall. Ex Roxb is widely distributed[1] in Yunnan, Guizhou province and Guangxi Zhuang Autonomous Region, China[1]. Its arial parts is used as traditional medicine for the treatment of hepatitis A and B[2]. Investigation on this plant led to the isolation of two new pentacyclic triterpenes. Their structures were established as 1α, 3β-dihydroxyl-olean-12-en-28-oic acid and 1α, 2α, 3β-trihydroxyl-olean-12-en-28- oic acid (**Figure 1**).

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



compound **1** compound **2**

Compound **1** was isolated as white powder, mp 212°C, $[\alpha]_D^{15}$ –23 (MeOH, c 0.001). HR-EIMS (found 472.3588, calcd. 472.3553) suggested the molecular formula as $C_{30}H_{48}O_4$. EIMS spectrum gave a molecular ion peak at *m/z* 472 $[M]^+$ (10) and fragment ion peaks at 454 (20), 436 (10), 248 (100), 203 (60). IR (KBr) showed

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absorptions at 3423 cm^{-1} (OH), 1696 cm^{-1} (C=O) and 1628 cm^{-1} (C=C). Seven singlet peaks in the high field of ^{1}H-NMR indicated that it was an oleanane triterpene. δ_C 72.8 and 71.8 revealed that there were 1 α, 3β-dihydroxyl groups on ring A[3]. A fragmental ion of EIMS at *m/z* 248 (100) resulting from retro-Diels-Alder cleavage of C-ring supported the assignment of two hydroxyl groups at the A/B rings. Rings A and B were determined by comparing the ^{13}C-NMR data with those of imberbic acid (1 α, 3β-dihydroxyl-olean- 12-en-29-oic acid)[4]. Rings C, D and E were the same as oleanolic acid by comparison with their ^{13}C-NMR data[3]. Therefore, compound **1** was identified as 1α, 3β-di hydroxyl-olean-12-en-28-oic acid, which was a new compound. ^{1}H-NMR （C_5D_5N, 300 MHz, δ ppm） 5.55 (brs, 1H, H-12,), 4.37 (dd, 1H, J = 10.8, 5.4 Hz, H-3), 3.83 (brs, 1H, H-1), 3.34 (dd, 1H, J = 13.1, 4.0 Hz, H-18), 2.93 (dd, 1H, J = 10.6, 5.8 Hz, H-9), 0.94, 1.01, 1.02, 1.11, 1.13, 1.33, 1.36 (7×-CH_3); ^{13}C-NMR (C_5D_5N, 75 MHz) δ 72.8 (C-1, d), 35.7 (C-2, t), 71.8 (C-3, d), 39.8 (C-4, s), 48.4 (C-5, d), 18.7 (C-6, t), 33.0 (C-7,t), 39.4 (C-8, s) 38.3 (C-9, d), 42.6 (C-10, s), 23.4 (C-11, t), 122.8 (C-12, d), 144.5 (C-13, s), 41.4 (C-14, s), 28.4 (C-15, t), 23.7 (C-16, t), 46.6 (C-17, s), 41.9 (C-18, d), 46.5 (C-19, t), 30.9 (C-20, s), 34.1 (C-21, t), 33.1 (C-22, t), 28.8 (C-23, q), 17.5 (C-24, q), 16.4 (C-25, q), 16.4 (C-26, q), 26.2 (C-27, q), 180.0 (C-28, s), 33.2 (C-29, q), 23.8 (C-30, q).

Compoud **2** was obtained as white powder, mp: 246°C, $[\alpha]_D^{15}$ –42 (MeOH, c 0.001). ESIMS indicated the quasi-molecular ion at *m/z* 489 $[M+H]^+$, HR-EIMS ion at m/z 488.3486 $[M]^+$, determined the molecular formula as $C_{30}H_{48}O_5$ (calcd. 488.3503) which was consistent with the ^{13}C and ^{1}H-NMR spectral data. IR showed absorptions at 3420 cm^{-1} (OH), 1694 cm^{-1} (C=O) and 1630 cm^{-1} (C=C). The ^{1}H-NMR spectrum exhibited the presence of seven angular methyl groups at δ 0.94，0.99，1.00，1.05，1.08，1.28，1.36 (each 3H, s), respectively. One carboxyl group at δ 179.6 (s) and two olefinic carbon signals at 122.2 (d) and 144.1 (s) in ^{13}C NMR were also observed. The above evidence suggested that compound **2** was an oleanane-type triterpenoid. Three proton signals at δ 3.93 (d, J = 2.8 Hz), 4.21 (dd, J = 10.0, 2.8 Hz) and 4.00 (d, 10.0 Hz), which coupled with each other, showed that three hydroxyl groups were located at C-1, C-2 and C-3, this was confirmed by the HMBC correlation between H-1 and C-2, C-3, C-5, H-2 and C-1, C-3, C-4, H-3 and C-2, C-4, C-23, C-24. The proton coupling constant showed that H-1 was equatorial, H-2 and H-3 were axial. NOESY correlation of H-1 and H-2, H-25, H-2 and H-1, H-24, H-25, H-3 and H-23 further corroborated the above conclusion (**Figure 2**). So compound **2** was elucidated to be 1α, 2α, 3β-trihydroxyl-olean-12- en-28-oic acid, and its ^{1}H and ^{13}C-NMR spectra (**Table 1**) were completely assigned by detailed 2D-NMR experiments.

Figure 2 The NOESY of compound **2**

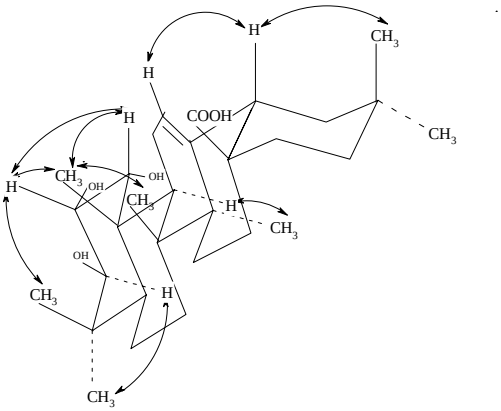

Table 1 The ^{1}H-(400MHz) and ^{13}C-(100MHz) NMR spectral data for compound **2** (pyridine-d_5, TMS)

C	δ_C	δ_H	HMBC
1	74.6 (d)	3.93 (1H, d, J = 2.8Hz)	C-2, 3, 5
2	70.0 (d)	4.21 (1H, dd, J = 10.0, 2.8Hz)	C-1, 3, 4
3	76.6 (d)	4.00 (1H, d, 10.0Hz)	C-2, 4, 23, 24
4	39.0 (s)		
5	47.6 (d)		
6	18.3 (t)		
7	32.6 (t)		
8	41.4 (s)		
9	38.0 (d)	2.93 (1H, dd, J = 10.8, 6.0Hz)	C-8, 10, 11, 25, 26
10	39.2 (s)		
11	22.9 (t)		
12	122.2 (d)	5.50 (1H, brs)	
13	144.1 (s)		
14	42.1 (s)		
15	29.4 (t)		
16	27.8 (t)		
17	46.1 (s)		
18	41.4 (d)	3.26 (1H, dd, J = 13.2, 4.0Hz)	C-19
19	45.9 (t)		
20	30.3 (s)		
21	33.6 (t)		
22	32.3 (t)		
23	28.7 (q)	1.36 (3H, s)	C-3, 4, 5, 24
24	16.6 (q)	1.05 (3H, s)	C-3, 4, 5, 23
25	17.1 (q)	1.08 (3H, s)	C-1, 5, 8, 9
26	15.6 (q)	1.00 (3H, s)	C-8, 9, 14
27	25.7 (q)	0.99 (3H, s)	C-8, 9, 13, 14, 15
28	179.6 (s)		
29	32.6 (q)	1.28 (3H, s)	C-19, 20, 21, 30
30	23.2 (q)	0.94 (3H, s)	C-19, 20, 21, 29

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