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Abietane Quinones from *Rabdosia serra*

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Abstract: A new abietane quinone diterpenoid was isolated, together with horminone, 16-acetoxy-7-0-acetylhorminone, β-sitosterol, stigmasterol, ursolic acid and palmitic acid from the leaves of *Rabdosia Serra (MAXIM) Hara*. The new compound was elucidated as 16-acetoxy-7α-ethoxyroyleanone.

Keyword: *Rabdosia Serra (MAXIM) Hara*, Labiatae, Abietane quinones.

Rabdosia Serra (MAXIM) Hara is a chinese traditional medicine for the treatment of hepatitis, enteritis, acute cholecystitis and dysentery[1]. The present communication describes the first isolation of three abietane quinone diterpenoids from the herb (**Figure 1**). The new abietane quinone, 16-acetoxy-7α-ethoxyroyleanone **1** was elucidated. In addition, two known abietane quinones, horminone **2**, 16-acetoxy-7-0-acetylhorminone **3** and β-sitosterol, stigmasterol, ursolic acid, palmitic acid were identified.

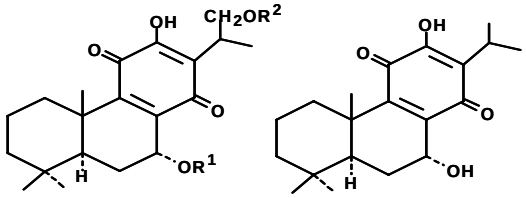
Results and discussion

Compounds **2, 3** were identified by comparison of their spectroscopic data (UV, IR, ^{1}HNMR, ^{13}CNMR and MS) with some of published compounds [2-3].

Compound **1** gave IR absorption bands for a characteristic quinonoid structure (1660, 1654, 1650, 1627, 1600 cm^{-1}) and which was further confirmed by the typical UV absorption maxima at 214 nm (ε: 7860) and 270 nm (ε: 9238)[2]. The ^{13}CNMR spectrum showed signals at δ: 186.11 (s), 183.87 (s), 151.62 (s), 148.33 (s), 142.01 (s), 120.19 (s) also indicated there was a quinonoid structure. **1** was assigned the molecular formula $C_{24}H_{34}O_6$ by MS (M+ at *m/z* 418) and ^{13}CNMR. The IR showed there were a hydroxy group (3370 cm^{-1}) and an ester group (1730 cm^{-1}, 1220 cm^{-1}) in the molecule. The UV, IR, ^{1}HNMR and ^{13}CNMR of **1** were very similar to those of **3**, and this suggested that **1** and **3** had the same structure skeleton and oxygenation pattern[3]. The ^{13}CNMR spectrum of **1** suggested that there were three carbon atoms attached to an oxygen respectively by single bond (69.42, 66.38, 65.67), and based on ^{1}HNMR and IR, there were an ethoxy group and an acetoxy group but no oxygen containing substitution on ring A [4], so it was supposed that one oxygen was located on ring B and the NOE experiment showed it's attachment to C_7[5]. The significant differences between **1** and **3**

were the absence of an ester group absorption in the IR and the disappearance of an acetoxy group signal in the ^{1}HNMR of the former. The presence of an ethoxy group of **1** caused the upfield shift of the signal for H-7β from δ 5.90 to δ 4.38. Thus **1** was determined as 16-acetoxy-7α-ethoxyroyleanone.

Figure 1



	R1	R2
1	Et	Ac
3	Ac	Ac

2

Experimental

R. serra leaves were collected in Fujian Province of China and identified by Prof. Huang Xingsheng, botanist at our institute where a voucher specimen has been deposited.

Dried and powdered leaves (4.8Kg) were extracted with EtOH and the solvent was evaporated. The residue was dissolved in MeOH and decolourized by active charcoal. The filtrate was concentrated and mixed with silica gel. The mixture was submitted to cc (silica gel) eluting with increasing proportions of Me_2CO-Petroleum ether. All fractions were yielded in order of increasing polarity: **2** (42mg), **3** (38mg), **1** (14mg), β-sitosterol (312mg), stigmasterol (630mg), palmitic acid (27mg), ursolic acid (2.1g).

Compound **1**. $C_{24}H_{34}O_5$, yellow needles. mp. 182-184°C; UV λ^{EtOH} nm (ε): 214 (7860), 270 (9238); IR (cm^{-1}): 3370, 1730, 1660, 1654, 1650, 1627, 1600, 1457, 1380, 1326; MS: *m/z* (70ev): 418$[M]^+$, 43(base peak); ^{1}HNMR (200MHz, $CDCl_3$): δ 2.67(1β, m), 4.39(7β, d), 7.19(12-OH, s), 3.36(15, sextet), 4.22(16, dd), 1.22(17-Me, d), 0.88(18-Me, s), 0.91(19-Me, s), 1.19(20-Me, s), 1.98(OAc, s), 3.35, 1.16(OCH_2CH_3, q, t); ^{13}CNMR (400MHz): δ 35.74 (C-1, t), 18.75 (C-2, t), 41.08 (C-3, t), 39.41 (C-4, s), 45.62 (C-5, d), 22.08 (C-6, t), 69.42 (C-7, d), 142.01 (C-8, s), 148.33 (C-9, s), 33.15 (C-10, s), 186.11 (C-11, s), 151.62 (C-12, s), 120.19 (C-13, s), 183.87 (C-14, s), 29.45 (C-15, d), 66.38 (C-16, t), 15.10 (C-17, q), 33.15 (C-18, q), 23.12 (C-19, q), 18.75 (C-20, q), 65.67 (OCH_2CH_3, t), 15.90 (OCH_2CH_3, q), 171.27 (COMe, s), 19.03 (COMe, q).

References

1. Jiangsu Medicine College, "*Dictionary of Chinese Medicine*", Shanghai People's Publishing House, Shanghai, China, **1977,** p. 2511
2. M. Hensch, P. Ruedi, C. H. Eugster, *Helv. Chim. Acta*, **1975**, *58*, 1921.
3. Y. L. Xu, Y. B. Ma, L. Zhou, and H. D. Sun, *Phytochemistry*, **1988**, *27*, 3681.
4. P. Ruedi, *Helv. Chim. Acta*, **1984**, *67*, 1116.
5. G. Y. Li, Y. L. Wang, W. Z. Song, *Acta Pharm. Sinica*, **1987**, *22*(4), 269.

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