A New 24, 30-Dinortriterpenoid from *Paeonia delavayi*

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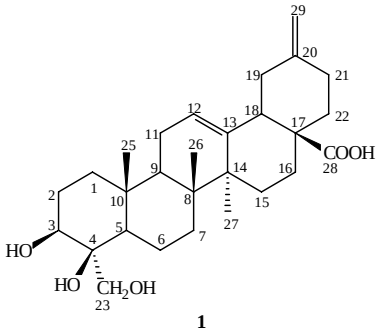
Abstract: A new triterpenoid, 3β, 4β, 23-trihydroxy-24, 30-dinorolean-12, 20(29)-dien-28-oic acid, together with five known compounds, 2α, 3β, 23-trihydroxy-12-oleanen-28-oic acid-β-D-glucopyranosyl ester, palbinone, 2-hydroxy-benzoic acid, vanillic acid, syringic acid, were isolated from the roots of *Paeonia delavayi* Franch. Their structures were characterized by spectral analysis.

Keywords: *Paeonia delavayi* Franch., Paeoniaceae, triterpenoid, 3β, 4β, 23-trihydroxy-24, 30-dinorolean-12, 20(29)-dien-28-oic acid.

We reported some constituents from the plant of *Paeonia delavayi* Franch[1]. Further investigation on the chemical constituents of the same plant resulted in the isolation and determination of a new triterpenoid, 3β, 4β, 23-trihydroxy-24, 30-dinorolean-12, 20(29)-dien-28-oic acid **1**, in addition to five known compounds, 2α, 3β, 23-trihydroxy-12-oleanen-28-oic acid-β-D-glucopyranosyl ester[2], palbinone[3], 2-hydroxy-benzoic acid[4], vanillic acid[4], syringic acid[5]. In this paper we describe the structural elucidation of the new compound.

Compound **1**, obtained as a white amorphous powder, was established to have a molecular formula of $C_{28}H_{42}O_5$ by EIMS at *m/z* 458 $[M]^+$ and ^{13}C NMR spectrum. The IR spectrum exhibited the presence of a hydroxyl group (3421 cm^{-1}), a carboxylic group (1719 cm^{-1}) and an exomethylene (1663 and 886 cm^{-1}). The ^1H and ^{13}C NMR spectra of **1** were very similar to those of 30-norhederagenin[6,7], except for the absence of the methyl group at C-24 and a quaternary carbon at about δ 40 ppm and the presence of a quaternary carbon at δ 75.6, which was attached to a hydroxyl group. In addition the ^{13}C NMR spectrum showed 28 carbon signals which suggested the dinor-skeleton of **1**. The ^1H NMR spectrum showed two protons at δ 4.79 (s) and 4.74 (s) due to the exomethylene protons of H-29, one proton at δ 4.30 (*dd*, J = 11.5, 5.2 Hz) assigned to H-3α, and two protons at δ 4.39 (*d*, J = 10.4 Hz) and 4.08 (*d*, J = 10.4 Hz) of H-23. In the HMBC spectrum, the cross-peaks from H-19 (δ 2.62 and 2.25) to C-20 [δ 149.0 (quaternary carbon)] and C-29 [δ 106.8 (CH_2)], and from H-29 (δ 4.79 and 4.74) to C-20 and C-19 [δ 41.8 (CH_2)], indicated that the exocyclic double bond was located between C-20 and C-29. Furthermore, the long-range couplings were also observed for H-3 (δ 4.30) to C-23 [δ 64.3 (CH_2)] and C-4 [δ 75.6 (quaternary carbon)], and for H-23 (δ 4.39 and 4.08) to C-4. The NOESY spectrum showed NOE interaction between H-3 and

H-23. Thus, the structure of compound **1** was determined as 3β, 4β, 23-trihydroxy-24, 30-dinorolean-12, 20(29)-dien-28-oic acid.



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Compound **1**, $[\alpha]_D^{24}$ +89.3 (*c* 0.252, CH_3OH); UV (MeOH) λ_{max} 204.5 nm; IR (KBr) ν 3421, 2936, 1719, 1690, 1663, 1465, 1443, 1382, 1295, 1046, 886 cm^{-1}; ^1H NMR (400 MHz, C_5D_5N, δ ppm): 5.52 (*br s*, 1H, H-12), 4.79 (*s*, 1H, H-29a), 4.74 (*s*, 1H, H-29b), 4.39 (*d*, 1H, *J* = 10.4 Hz, H-23a), 4.30 (*dd*, 1H, *J* = 11.5, 5.2 Hz, H-3), 4.08 (*d*, 1H, *J* = 10.4 Hz, H-23b), 3.24 (*dd*, 1H, *J* = 13.6, 4.6 Hz, H-18), 2.62 (*t*, 1H, *J* = 13.5 Hz, H-19β), 2.25 (overlap, 1H, H-19α), 1.79 (*d*, 1H, *J* = 10.8 Hz, H-9), 1.68 (*d*, 1H, *J* = 11.2 Hz, H-5), 1.37 (*s*, 3H, H-25), 1.20 (*s*, 3H, H-27), 1.11 (*s*, 3H, H-26); ^{13}C NMR (100 MHz, C_5D_5N, δ ppm): 38.5 (C-1), 27.1 (C-2), 71.1 (C-3), 75.6 (C-4), 48.1 (C-5), 18.3 (C-6), 32.8 (C-7), 39.7 (C-8), 47.2 (C-9), 36.9 (C-10), 23.6 (C-11), 123.1 (C-12), 144.1 (C-13), 42.2 (C-14), 28.2 (C-15), 23.6 (C-16), 46.9 (C-17), 47.9 (C-18), 41.8 (C-19), 149.0 (C-20), 30.2 (C-21), 38.2 (C-22), 64.3 (C-23), 15.6 (C-25), 17.6 (C-26), 26.1 (C-27), 179.2 (C-28), 106.8 (C-29); EIMS (70 eV) *m/z* (%): 458 $[M]^+$ (9), 427 (45), 412 (5), 248 (12), 232 (100), 204 (23), 187 (98), 173 (35), 159 (30), 131 (37), 105 (46), 91 (45).

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