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# New antibacterial triterpenoid saponin from *Lactuca scariola*

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## Abstract

A new antibacterial triterpenoid saponin, 3β-*O*-[α-L-rhamnopyranosyl]-30-norolean-12,19-diene-28-oic acid 28-*O*-[β-D-glucopyranosyl-(1→4)-*O*-β-D-galactopyranosyl]-ester (**1**); has been isolated from the stems of *Lactuca scariola*. Its structure was determined by chemical degradations and spectral analysis.

*Keywords: Lactuca scariola*; Triterpenoid saponin; Antibacterial activity

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## 1. Introduction

*Lactuca scariola* [1–3] is commonly known as “Kahu” in Hindi. It is widely distributed in W. Himalaya up to 6000–12,000 ft. The leaves of this plant are useful as stomachic, to purify the blood, cure biliousness, in burning sensation, headache, troubles of the nose, bronchitis and cough. Its seeds are used in the treatment of headache, ophthalmia and relieve inflammation. It is also used as analgesic, hypnotic and to prevent the fall of hair. Earlier workers [4–6] have reported the presence of various constituents from this plant.

In the present paper we report the isolation and structural elucidation of a new antibacterial triterpenoid saponin 3β-*O*-[α-L-rhamnopyranosyl]-30-norolean-12,19-diene-28-oic acid-28-*O*-[β-D-glucopyranosyl-(1→4)-*O*-β-D-galactopyranosyl] ester (1) from the stems of *L. scariola* on the basis of chemical degradations and spectral analysis.

## 2. Experimental

### 2.1. General

Melting points: Thiel’s apparatus. $^1$H-NMR spectra were recorded at 300 MHz, in $CDCl_3$, $^{13}$C-NMR spectra at 90 MHz, in DMSO-$d_6$. Mass spectra: Jeol D-300.

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### 2.2. Plant

*Lactuca scariola* L.(Compositae), stems supplied by M/S United Chemical and Allied Products, Kolkata were taxonomically identified by the Taxonomist, Department of Botany, Dr. H.S. Gour University, Sagar (M.P.). The voucher specimen was deposited in the Chemistry Department of Dr. H.S. Gour University.

### 2.3. Extraction and isolation of compound 1

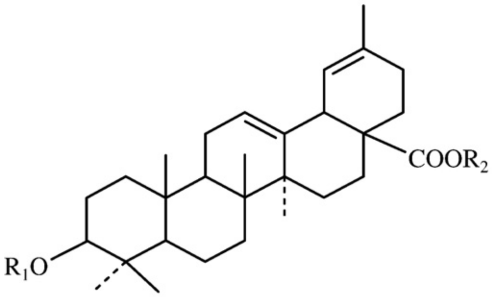
Dried powdered stems (4 kg) were Soxhlet extracted with 95% EtOH yielding a brown viscous extract, successively partitioned with petroleum ether (40–60 °C), $CHCl_3$, EtOAc, acetone and MeOH. The acetone fraction was concentrated in vacuo giving a light brown amorphous mass. It gave a precipitate on addition of excess $Et_2O$. The precipitate was Si-gel CC with MeOH–$CHCl_3$ giving compound **1** (1.75 g).

Compound (**1**, Fig. 1), mp 260–262 °C (MeOH); [$M^+$] 910 (FABMS) (found C; 62.01%, H; 8.21%, calcd. for m.f. $C_{47}H_{74}O_{17}$, C; 61.98%, H; 8.13%) ; IR bands (KBr) 3424, 2937, 1722, 1436, 1383, 1241, 1210, 1115, 1032, 998, 830, 755cm$^{-1}$; FABMS $[M]^+$, *m/z*:910, 764, 748, 602, 586, 440, 425, 422, 395, 377, 233, 219, 207, 189, 187, 162, 133. Calc. for $C_{47}H_{74}O_{17}$. $^{13}$C-NMR: see Table 1.

Compound **1** decaacetato ($Ac_2O$-pyr), mp 194–196 °C; [M] 1330; $^1$H-NMR (300 MHz, $CDCl_3$): δ 0.74, 0.78, 0.93, 0.97, 1.06, 1.54 (18H, s, 6 × Me), 3.28 (2H, m, H-3 and H-18), 5.07 (1H, brs, H-19), 5.48 (1H, t, *J* 3.8Hz, H-12), 5.48 (1H, d, *J* 3.7Hz, H-1′), 4.65 (1H, dd, *J* 3.7, 9.7Hz, H-2′), 4.58 (1H, dd, *J* 9.7, 3.3Hz, H-3′), 4.60 (1H, d, *J* 3.1Hz, H-4′), 4.63 (1H, m, H-5′), 4.40 (2H, d, *J* 6.3Hz, H-6′), 4.45 (1H, d, *J* 7.7Hz, H-1″), 2.92–3.12 (4H, m, H-2″, H-3″, H-4″, H-5″), 3.91 (2H, dd, *J* 2.4, 4.6Hz, H-6″), 5.26 (1H, brs, H-1‴), 3.90 (1H, d, *J* 2.5Hz, H-2‴), 3.81 (1H, dd, *J* 2.2, 9.3Hz, H-3‴), 3.41 (1H, dd, *J* 9.1, 8.9Hz, H-4‴), 3.46 (1H, dd, *J* 9.4, 5.8Hz, H-5‴), 1.28 (3H, d, *J* 6.1Hz, H-6‴), 2.06–2.16 (9H, m, 3 × OAc), 2.05 (6H, s, 2 × OAc), 1.98 (3H, s, OAc), 2.02 (3H, s, OAc), 2.31 (3H, s, OAc), 2.16 (3H, s, OAc), 2.25 (3H, s, OAc).

#### 2.3.1. 3β-Hydroxy-30-norolean-12,19-dien-28-oic acid (2)

Compound **1** (450 mg) was refluxed with 10% EtOH $H_2SO_4$ on a water bath for 8 h. The reaction mixture was concentrated in vacuo and allowed to cool. The residue was extracted with $Et_2O$. The aqueous layer was worked-up separately for identification of sugars. The ethereal layer was washed with water and evaporated to dryness, to yield compound **2** (325 mg), $C_{29}H_{44}O_3$, mp 241–243 °C, [$M^+$] 440 (FABMS); IR bands (KBr) 3423, 2939, 1717, 1438, 1388, 1240, 1212, 1110, 1035, 1004, 825, 750cm$^{-1}$; $^1$H-NMR (300 MHz, $CDCl_3$): δ 0.76, 0.81, 0.90, 0.98, 1.04, 1.56 (18H, s, 6 × Me), 3.26 (2H, m, H-3 and H-18), 5.10 (1H, br, s, H-19), 5.44 (1H, t, *J* 3.8Hz, H-12); MS: [$M^+$] *m/z* : 440, 425, 422, 395, 377, 233, 219, 207, 189, 187, 162, 133.).



| | $R_1$ | $R_2$ |
|---|---|---|
| **1** | α-L-rha[a] | β-D-glu[b]-(1→4)-O-β-D-gal[c] |
| **2** | H | H |
| **3** | α-L-rha | H |

[a]rha = rhamnose, [b]glu = glucose, [c]gal = galactose

Fig. 1.