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A TRITERPENE ACID CONSTITUENT OF *SALVIA LANATA**

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Key Word Index—*Salvia lanata*; Labiatae; 3-epi-ursolic acid.

Abstract—The petrol extract of the whole plant (aerial parts and roots) of *Salvia lanata* yielded a new triterpene acid, 3-epi-ursolic acid.

In a previous communication [1] we reported the isolation and characterization of some diterpenoid quinones from the petrol extract of the whole plant (aerial parts and roots) of *Salvia lanata*. This paper reports the isolation and structure elucidation of a new pentacyclic triterpene acid, 3-epi-ursolic acid (**1**) from the petrol extract of the whole plant of *S. lanata*.

3-Epi-ursolic acid, $C_{30}H_{48}O_3$ (M^+, *m/z* 456), mp 240–245°, $[\alpha]_D + 98°$ ($CHCl_3$) gave a positive Liebermann–Burchardt test and its IR spectrum exhibited absorption bands at ν_{max}^{KBr} 3400 (hydroxyl), 1690 (carboxyl) and 1645 cm^{-1} (unsaturation). It formed an amorphous acetate, $C_{32}H_{50}O_4$ (**2**) with acetic anhydride and pyridine at room temperature and afforded a methyl ester, $C_{31}H_{50}O_3$ (**3**), mp 185–190°, with diazomethane. The ^1H NMR spectrum (100 MHz, $CDCl_3$) of the acid showed resonances for five tertiary methyls δ 0.60 (3H, *s*), 0.65 (3H, *s*), 0.75 (6H, *s*) and 1.21 (3H, *s*); two secondary methyls appearing as doublets around δ 1.03 (6H, $J = 6$ Hz); one vinylic proton at δ 5.30 (1H, *m*); and one proton multiplet around δ 4.38 assignable to > CHOH as expected for the urs-12-ene skeleton with a hydroxyl substituent. The mass spectrum of this triterpene was strikingly similar to that of ursolic acid [2] and exhibited peaks at *m/z* 456 $[M]^+$, 411 $[M - COOH]^+$, 248 (base peak), 207, 203 $[248 - COOH]^+$, 202 $[248 - HCOOH]^+$ and 189 $[207 - H_2O]^+$.

Further elaboration of the structure (**1**) of the triterpene was possible from its conversion to ursonic acid (**5**) [3] by chromic acid oxidation of its methyl ester followed by hydrolysis.

Conclusive evidence in favour of the axial (α) orientation of the C-3 hydroxyl was obtained from the ^1H NMR spectrum (100 MHz, $CDCl_3$) of **2** which disclosed the presence of a triplet-like single proton signal centred at δ 5.45 with a splitting pattern typical of a 3α-acetoxyl group [4]. Other peaks were observed at δ 5.29 appearing as a broad multiplet for a vinylic proton, a singlet of three protons at δ 2.04 assignable to an acetoxy methyl and several peaks in the region δ 0.80–1.45 for methyl and methylene protons.

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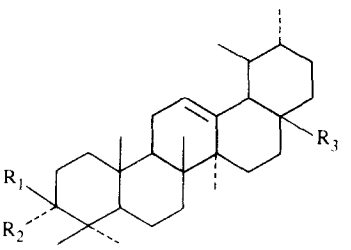

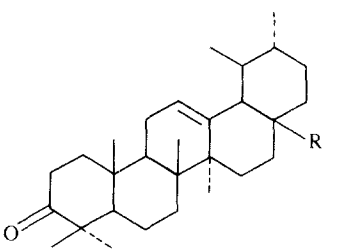

1 $R_1 = H$, $R_2 = OH$, $R_3 = COOH$

2 $R_1 = H$, $R_2 = OAc$, $R_3 = COOH$

3 $R_1 = H$, $R_2 = OH$, $R_3 = COOMe$

4 $R = COOMe$

5 $R = COOH$

EXPERIMENTAL

All mps are uncorr.

Extraction of Salvia lanata. *Ca* 1 kg air dried, finely powdered whole plant (aerial parts and roots) of *Salvia lanata* Roxb. was extracted with petrol (60–80°) in a Soxhlet for 48 hr. The extract was subjected to CC on 200 g Si gel (mesh 60–120). Fractions 178–187 were collected.

Isolation of 3-epi-ursolic acid (**1**). Fractions 178–187 yielded 3-epi-ursolic acid. It crystallized from EtOAC–petrol (40–60°; 1:3), yield 0.35 g, mp 240–245°, $[\alpha]_D + 98°$ ($CHCl_3$). IR ν_{max}^{KBr} cm^{-1}: 3400 (OH), 2920, 1690, 1645, 1440, 1380, 1270, 1020, 985 and 660. ^1H NMR ($CDCl_3$) and MS: described in the text.

Acetylation of 3-epi-ursolic acid. 3-Epi-ursolic acid (50 mg) was dissolved in 5 ml Ac_2O and 0.5 ml C_5H_5N and the reaction mixture was kept at room temp. for 4 days. The reaction mixture was then poured into cold H_2O, extracted with Et_2O and dried when the amorphous acetate **2** was obtained (yield 56 mg) IR ν_{max}^{KBr} cm^{-1}: 2948, 1735 (acetyl), 1695 (carboxyl), 1640 (unsaturation). ^1H NMR (100 MHz, $CDCl_3$): described in the text.

Methyl ester of 3-epi-ursolic acid (**3**). 3-Epi-ursolic acid (50 mg) dissolved in MeOH and methylated with excess CH_2N_2 in Et_2O at 5°, crystallized from $CHCl_3$–MeOH (1:1), mp 185–190°. IR ν_{max}^{KBr} cm^{-1}: 3450 (OH), 1725 (ester carboxyl), 1645 (unsaturation).

Jones' oxidation of **3**. The methyl ester (**3**, 50 mg) was dissolved in 20 ml glacial HOAc and to it a soln of chromic acid (20 mg) in 5 ml glacial HOAc was added. The mixture was refluxed for nearly 2 hr at 50°, cooled, filtered and the filtrate was acidified with moderately conc. HCl in the cold. The ppt was dissolved in Et_2O, dried and the Et_2O removed to leave a crude solid which on repeated CC over 50 g Si gel (mesh 60–120) furnished the methyl ester of ursonic acid (**4**), mp 190–193°, $[\alpha]_D + 84°$ ($CHCl_3$) crystallized from $CHCl_3$–MeOH (1:1).

Alkaline hydrolysis of **4**. Methyl ursonate (**4**, 25 mg) was dissolved in 10 ml 20% ethanolic KOH and refluxed for 8 hr, solvent removed, H_2O added and the mixture filtered. The filtrate was acidified with HCl and extracted with Et_2O. The extract was washed with H_2O until free from acid, dried and the solvent distilled to leave ursonic acid, $C_{30}H_{46}O_3$ (**5**), mp 272–276° (d), $[\alpha]_D + 80°$ ($CHCl_3$) crystallized from MeOH.

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AMASTEROL, AN ECDYSONE PRECURSOR AND A GROWTH INHIBITOR FROM *AMARANTHUS VIRIDIS*

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Key Word Index—*Amaranthus viridis*; Amaranthaceae; sterol; ecdysone precursor; growth inhibitor.

Abstract—A sterol isolated from the roots of *Amaranthus viridis* has been assigned the structure 24-methylene-20-hydroxycholest-5,7-en-3β-ol.

INTRODUCTION

Several ecdysteroids have been isolated from members of the Amaranthaceae. The genus *Amaranthus* has been found to elaborate β-ecdysone [1] and inokosterone [2] while from *Cyathula*, amarasterone and amarasterone B [3] were isolated. While investigating the chemical constituents of Indian medicinal plants, our interest was directed to the genus *Amaranthus* which is cultivated in India as a crop. We now report the isolation of a new growth inhibitory steroid amasterol from the petroleum ether extract of the roots of *Amaranthus viridis L.*